AJMS
Asian Journal of Mathematical Sciences

REVIEW ARTICLE

ON DIFFERENT METHODS OF ESTIMATING CORRELATION COEFFICIENTS

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Received: 15-01-2026; Revised: 09-02-2026; Accepted: 25-03-2026

ABSTRACT

Correlation analysis uses different methods to measure the extent of relationship between two variables. Different methods of estimating correlation coefficients have been used by various researchers, but the challenge has been using the appropriate methods. In this study, fourteen different methods of estimating correlation coefficients were examined with emphasis on their assumptions, properties and relationships existing among some of the methods. While derivations were made of Pearson's correlation with its limit; Spearman's correlation; Biserial and Point Biserial, Kendall's Tau by neighbor swaps was illustrated with order of performance of numeric data. The relationships among the methods examined showed that Phi coefficient has similar relation with Tetrachoric as Point Biserial relates with Biserial correlation coefficient. It was also established that Pearson's correlation assesses linear relationship between variables, but Spearman' rank correlation assesses monotonic relationship. Statistical applications of the methods to real life situations were also established.

Keywords: Correlation Coefficient, Concurrent Deviations, Tetrachoric Correlation, Point Biserial Correlation, Yule's Correlation Coefficient.

INTRODUCTION

Correlation analysis is a statistical technique or bivariate that measures the magnitude and direction of linear relationship between two variables[1]. For example, degree of overcrowding and prevalence of pulmonary tuberculosis are correlated; severity of malnutrition is well correlated with the severity of pulmonary tuberculosis; economic status and health status are well correlated; ageing and blood pressure are positively correlated; degree of adiposity and cholesterol levels are also positively correlated[2]; intake of calories and proteins are positively correlated and economic status and the quantities of sorghum consumed (Rao and Sinharay, 2007). There are different methods of estimating correlation coefficients, some of which are parametric and others nonparametric[3]. Over the years, there have been misconceptions on whether or not a particular method is suitable to measure a linear relationship between two variables[4]. In addition to this, many researchers often utilize inappropriate correlation methods in the study of linear relationships which usually lead to unreliable and invalid results (Washington, 2010). The accuracy of correlation coefficients' estimation has been a serious challenge among researchers in recent times. This may be due to insufficient knowledge on the methods of correlation coefficients and the associated assumptions which eventually result to undue usage of correlation coefficient methods in research analysis (Winter and Gosling, 2016).

Etaga et al (2021) investigated some five methods of estimating correlation coefficients in the presence of influential outliers[5]. The researchers compared five methods and concluded that Pearson's method was appropriate when data are non-contaminated and other methods could be used for contaminated data.

Makowski et al (2020) presented correlation as a tool for R language and part of the easy stats collection that was focused on correlation analysis. The researchers aimed at light weighting, easy to use and allows for the computation of different types of correlations[6]. In this study, fourteen different methods of estimating correlation coefficients along with their assumptions, properties and relationships among them are examined with some of the methods derived.

Preliminaries and Definitions

In this section, we introduce classification of correlations, spectrum of interpreting correlation coefficients, definition of correlation coefficient and avoidable errors when interpreting correlation coefficients[7].

1.1: Classification of Correlations

Classification of correlations is based on the direction of change, number of variables and constancy of the ratio between the variables under consideration (Kozak, 2008).

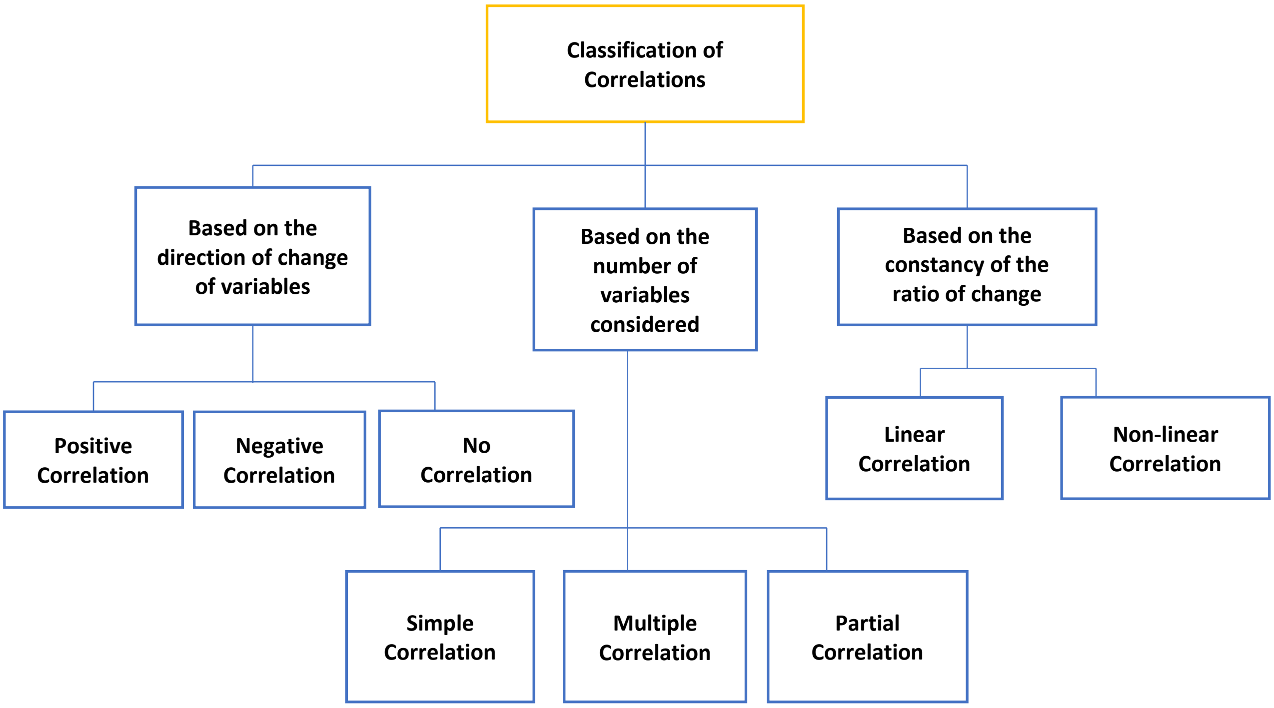


Figure 1: Classification of Correlation Coefficients

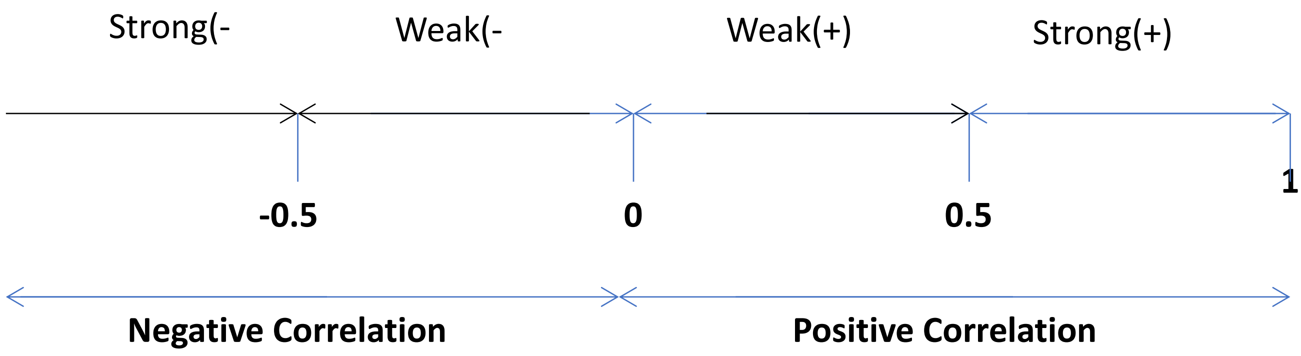


Figure 2: Spectrum of Interpreting Correlation Coefficients

1.2: Properties of Correlation Coefficients

The correlation coefficient r has the following properties:

(i) The limit

(ii) r is independent of change of origin and scale

(iii) Two independent variables are uncorrelated, but the converse is not true

(iv) Given that two variables X and Y are related by mX + nY = 0, then the correlation coefficient between X and Y is positive if m and n have different signs and negative and the signs of m and n are the same (Awogbemi and Oguntade, 2023).

1.3: Definitions of Some Terms used In Correlation Analysis

Coefficient of Correlation: Coefficient of correlation between two variables is a measure of linear relationship between the variables which indicates the amount of variation of one variable that is accounted for by another variable.

Positive Correlation: Two variables are positively correlated if they tend to increase and decrease together in the same direction.

Negative Correlation: Two variables are positively correlated if they tend to increase and decrease together in opposite direction.

Zero Correlation: Two variables are uncorrelated (no correlation) if they tend to change with no definite relationship or connection to each other.

Coefficient of Determination: This is a correlation measure that gives the percentage variation in the dependent variable that is accounted for by the independent variable. In other words, coefficient of determination denoted by r^2 indicates the ratio of the explained variance to the total variance.

Coefficient of Non-determination: This is the ratio of the unexplained variation to total variation and it is denoted by $K^2 = 1 - r^2$. The higher the value of unexplained variance, the poorer the efficiency of the other variable estimated.

Coefficient of Alienation: This is the square root of coefficient of non- determination and it is denoted by

$$K = \pm\sqrt{1 - r^2}$$

Linear Correlation: The correlation between two variables is said to be linear if corresponding to a unit change in one variable, there is a constant change in the other variable over the entire range of the values.

Non-linear or Curvilinear Correlation: The correlation between two variables is said to be non-linear if corresponding to a unit change in one variable, the other variable does not change at a rate, but at a fluctuating rate.

Bi-weight mid-correlation: This is a measure of similarity that is median based instead of the traditional mean-based correlation. It is thus less sensitive to outliers (Lanfelder and Hryath, 2012).

Percentage Bend Correlation: This is based on a down-weight of a specified percentage of marginal observations deviating from the median.

Distance Correlation: This measure both linear and nonlinear relationships between two random variables or vectors.

Shephered's Pi Correlation: This is similar to Spearman's rank correlation after removing the outliers using bootstrapped Mahalanobis distance.

Polychoric Correlation: This correlation measures the correlation between two theorized normally distributed continuous variables from two observed variables.

Tetrachoric Correlation: This is a special type of the correlation coefficient

that is used when two observed variables are artificially dichotomous.

Partial Correlation: This is correlation in which more than two variables are recognized, only two variables influencing each other are considered, while the effect of other influencing variables is being kept constant.

Multilevel Correlations: These are special types of partial correlation where the variable to be adjusted for is a factor and is included as a random effect in a mixed model.

Interpretation of Correlation Coefficients

The interpretation of a correlation coefficient is purely mathematical and completely devoid of any cause or effect implication[8]. For instance, if two variables tend to increase or decrease together, it does not mean that one has any direct or indirect effect on the other. The two variables may be influenced by other variables in such a way as to give rise to a strong relationship[9]. Therefore, correlation coefficient must be handled with caution if they are expected to give sensible information concerning relationships between pairs of variables (Rao, 2007). The most commonly avoidable errors when interpreting correlation coefficients are identified and remedial measures are specified below:

Table 1: Commonly Made Errors when Interpreting Correlation Coefficients and

Remedial Measures

	Common Errors when Interpreting Correlation Coefficients	Remedy Measures
	Misinterpreting correlation as causation: That Two variables are correlated does not imply one causes the other. A correlation between smoking and cancer is not enough to say that smoking causes cancer.	To establish causation, conduct experiments, use statistical methods that control for confounding and test for significance.

(b)	Sample size of observations: Larger sample size provides more reliable coefficient estimates, but small sample size may lead to a high correlation coefficient due to chance.	To avoid this error, always use appropriate and consistent scales bearing in mind their limitations and assumptions.
(c)	Applying correlation coefficients to inappropriate or insufficient data: A correlation coefficient is only valid and significant if it satisfies certain criteria and assumptions.	To avoid this error, always check and establish the quality and suitability of data before applying and interpreting correlation coefficients.
(d)	Ignoring shapes and outliers of data points: Correlation coefficient only measures the magnitude and direction of a linear relationship, but does not capture the curvature, clustering or outliers of the data.	To overcome this pitfall, always use scatter plots to visualize data and check for nonlinearity.
(e)	Use of misleading scales for variables.	To avoid this error, use appropriate and consistent scales for variables under consideration and also noting the limitations and assumptions of the scales.
(f)	Simpson's paradox: Aggregating data can lead to paradoxical results. For example, aggregate marks versus marks in one subject.	Avoid a relationship between a variable and one of its components (subgroups).

Methods of Estimating Correlation Coefficients

Scatter Diagram Method

This method otherwise known as Galton's graph gives a qualitative picture on how well a given line or curve describes the relationship between variables (Galton, 1889). It does not give a quantitative measurement of the correlation between variables, but it is rather based on individual observation of the scattered plots (Aliyu, 2023) [10]. The scatter points can lie close to a line (positive or negative slope) to form a linear association; haphazard in nature and lie on a curve or very close to a curve to form a non-linear association. The downside of scatter diagram method is that it only provides the nature of existing relationship between variables without recourse to an exact measure of the extent of the relationship (Gupta, 2011) [11].

Pearson's Correlation Coefficient Method

$$r = \frac{S_{xy}}{\sqrt{S_{xx}S_{yy}}} = \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2 \sum_{i=1}^{n}(y_i-\bar{y})^2}}$$

Equation (1) is rewritten in a compact form as:

$$r = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{\sqrt{n\sum_{i=1}^{n} x_i - (\sum_{i=1}^{n} x_i)^2 n \sum_{i=1}^{n} y_i - (\sum_{i=1}^{n} y_i)^2}}$$

Alternatively, r is denoted by rxy and defined as the ratio of covariance between X and Y to the product of their individual standard deviations:

$$r_{XY} = \frac{Cov(x,y)}{\sigma_x \sigma_y}$$

If (x1,y1), (x2,y2), … ,(xn,yn) are n pairs of observations of X and Y in a bivariate, then

$$_{XY} = \frac{\frac{1}{n}\sum(x-\bar{x})(y-\bar{y})}{\sqrt{\frac{1}{n}\sum(x-\bar{x})^2 \frac{1}{n}\sum(y-\bar{y})^2}} = \frac{\sum(x-\bar{x})(y-\bar{y})}{\sqrt{\sum(x-\bar{x})^2\sum(y-\bar{y})^2}}$$

Proof:

Equation (2) is proved as follows:

$$r_{XY} = \frac{n\sum xy - \left(\sum x\right)\left(\sum y\right)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}$$

$$= \frac{\sum dxdy}{\sqrt{\sum dx^2 dy^2}}$$

Simplifying the numerator of equation (4), we have

$$\begin{aligned}
\text{cov}(x,y) &= \frac{1}{n}\sum(x-\bar{x})(y-\bar{y}) = \frac{1}{n}\sum(xy - \bar{x}y - x\bar{y} + \bar{x}\bar{y}) \\
&= \frac{1}{n}\sum xy - \bar{x}.\frac{1}{n}\sum y - \bar{y}.\frac{1}{n}\sum x + \frac{1}{n}.n\bar{x}\bar{y} \\
&= \frac{1}{n}\sum xy - \bar{x}\bar{y} - \bar{y}\bar{x} + \bar{x}\bar{y} \\
&= \frac{1}{n}\sum xy - \bar{x}\bar{y} \qquad (7) \\
&= \frac{1}{n}\sum xy - \left(\frac{\sum x}{n}\right)\left(\frac{\sum y}{n}\right)
\end{aligned}$$

$$= \frac{1}{n^2}\left[n\sum xy - \left(\sum x\right)\left(\sum y\right)\right] \qquad (8)$$

$$\sigma_x^2 = \frac{1}{n}\sum\left(x-\bar{x}\right)^2$$

$$= \frac{1}{n}\sum x^2 - \bar{x}^2 \quad ***$$

$$= \frac{1}{n}\sum x^2 - \left(\frac{\sum x}{n}\right)^2$$

$$= \frac{1}{n^2}\left[n\sum x^2 - \left(\sum x\right)^2\right] \qquad (9)$$

Similarly,

$$\sigma_y^2 = \frac{1}{n^2}\left[n\sum y^2 - \left(\sum y\right)^2\right]$$

Substituting equations (8), (9) and (10) in equation (3), we have

$$r_{XY} = \frac{\frac{1}{n^2}[n\sum xy - (\sum x)(\sum y)]}{\sqrt{\frac{1}{n^2}[n\sum x^2 - (\sum x)^2]\frac{1}{n^2}[n\sum y^2 - (y)^2]}}$$

$$= \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (y)^2]}}$$

Assumptions for Pearson's Correlation Coefficient

(i) The variables used for computation are continuous and scales of measurement are interval and ratio.

(ii) The distribution of variables is uni-modal and non-normal.

(iii) The pairs of observations are independent.

(iv) There is a linear relationship between two variables (Veeraraghavan and Shetgovekar, 2016)

Establishing the Limit of Pearson's Correlation Coefficient

Proof:

$$\sum\left(\frac{x-\bar{x}}{\sigma_x} \pm \frac{y-\bar{y}}{\sigma_y}\right)^2 \geq 0$$

$$=> \sum\left[\left(\frac{x-\bar{x}}{\sigma_x}\right)^2 + \left(\frac{y-\bar{y}}{\sigma_y}\right)^2 \pm 2\left(\frac{x-\bar{x}}{\sigma_x}\right)\frac{y-\bar{y}}{\sigma_y}\right] \geq 0$$

$$=> \frac{\sum(x-x)^2}{\sigma_x^2} + \frac{\sum(y-y)^2}{\sigma_y^2} \pm \frac{2\sum(x-x)(y-y)}{\sigma_x\sigma_y} \geq 0$$

Dividing equation (15) by n, we have

$$\frac{1}{\sigma_x^2}.\frac{1}{n}\sum(x-x)^2 + \frac{1}{\sigma_y^2}.\frac{1}{n}\sum(y-y)^2 \pm \frac{2}{\sigma_x\sigma_y}.\frac{1}{n}\sum\left(x-\bar{x}\right)\left(y-\bar{y}\right) \geq 0$$

$$=> \frac{1}{\sigma_x^2}.\sigma_x^2 + \frac{1}{\sigma_y^2}.\sigma_y^2 \pm \frac{2}{\sigma_x\sigma_y}Cov(x,y) \geq 0$$

$$|\Rightarrow 2+2r \geq 0 \quad or \quad 2-2r \geq 0$$
$$\Rightarrow -1 \leq r \quad or \quad r \leq 1$$
$$\Rightarrow -1 \leq r \leq 1$$

Spearman's Rank Correlation Coefficient Method

Spearman's Rank Correlation Coefficient was derived from the Pearson Moment Correlation Coefficient by replacing the actual observations by their ranks (Spearman, 1904). The method is used when dealing with qualitative characteristics that cannot be measured quantitatively, but can be arranged serially. The usage of this method brings about loss of information and is not practicable in the case of bivariate frequency distribution. This method is characterized by a non-parametric measure, non-normality, measured on ordinal scale and it is not affected by outliers.

Assumptions for Spearman's Rank Correlation

(i) The variables are measured in terms of ordinal scale

(ii) The relationship between the two variables is linear

(iii) Samples selected are random

(iv) The pairs of observations are independent (Mangal, 2002; Awogbemi and Oguntade, 2023; Oyeyemi et al, 2025).

Derivation of Spearman's Rank Correlation

The derivation of Spearman's Rank Correlation originated from Pearson's correlation coefficient\\\

$$r_{XY} = \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (y)^2]}} \qquad (19)$$

with the actual observations replaced by their respective ranks (assuming no ties) before computing the totals, sum of squares and cross products and n is the number of pairs observation while the difference of the paired ranks.

Proof:

$$\sum X_i = \sum R(X_i) = 1+2+...+n = \frac{n(n+1)}{2} \qquad (20)$$

$$\sum Y_i = \sum R(Y_i) = 1+2+...+n = \frac{n(n+1)}{2} \qquad (21)$$

Also,

$$\sum X_i^2 = \sum [R(X_i)]^2 = 1^2 + 2^2 + ... + n^2 = \frac{n(n+1)(2n+1)}{6} \qquad (22)$$

Similarly,

$$\sum Y_i^2 = \sum [R(Y_i)]^2 = 1^2 + 2^2 + ... + n^2 = \frac{n(n+1)(2n+1)}{6} \qquad (23)$$

By expansion,

$$\sum d_i^2 = \sum [R(X_i) - R(Y_i)]^2 = \sum [R(X_i)]^2 + \sum [R(Y_i)]^2 - 2\sum [R(X_i)][R(Y_i)] \qquad (24)$$

From equation (29),

$$\sum [R(X_i)][R(Y_i)] = \frac{1}{2}[\sum [R(X_i)]^2 + \sum [R(Y_i)]^2 - \sum [R(X_i) - R(Y_i)]]^2 \qquad (25)$$

Therefore,

$$\sum X_i Y_i = \sum [R(X_i)][R(Y_i)] = \frac{1}{2}[\frac{n}{3}(n+1)(2n+1) - \sum d_i^2] \quad (26)$$

$$r_s = \frac{\frac{n}{2}[\frac{n}{3}(n+1)(2n+1) - \sum d_i^2] - \frac{n^2(n+1)^2}{4}}{\left[\sqrt{\frac{n^2(n+1)(2n+1)}{6} - \frac{n^2(n+1)^2}{4}}\right]} \quad (27)$$

$$= \frac{\frac{n}{6}[(n+1)(2n+1) - 3\sum d_i^2] - \frac{n^2(n+1)^2}{4}}{\frac{n^2(n+1)(2n+1)}{6} - \frac{n^2(n+1)^2}{4}} \quad (28)$$

Multiplying the numerator and denominator of equation (28), we have

$$r_S = \frac{2n[n(n+1)(2n+1) - 3\sum d_i^2] - 3n^2(n+1)^2}{2n^2(n+1)(2n+1) - 3n^2(n+1)^2} \quad (29)$$

$$= \frac{2[n(n+1)(2n+1) - 3\sum d_i^2] - 3n(n+1)^2}{2n(n+1)(2n+1) - 3n(n+1)^2} \quad (30)$$

$$= \frac{2n(n+1)(2n+1) - 6\sum d_i^2 - 3n(n+1)^2}{2n(n+1)[(2n+1) - 3n(n+1)^2} \quad (31)$$

$$= \frac{n(n+1)2(2n+1) - 3(n+1) - 6\sum d_i^2}{n(n+1)[2(2n+1) - 3(n+1)]} \quad (32)$$

$$= \frac{n(n+1)(n-1) - 6\sum d_i^2}{n(n+1)(n-1)} \quad \vdots \quad (33)$$

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)} \quad (34)$$

Remark

Concurrent Deviations Method

This method determines the correlation between two series when we are not very concerned about the precision. The method is also based on the signs of the deviations of the values of the variable from its preceding value and does not consider the exact magnitude of the values of the variables. According to Gupta (2011), concurrent correlation coefficient is defined by

$$r = \pm\sqrt{\pm\left(\frac{2c-n}{n}\right)}, \quad (35)$$

where c is the number of pairs of concurrent deviations and n is the number of pairs of deviations.

Remarks:

If (2c-n) is positive, apply positive sign in and outside the square root in equation (35)

If (2c-n) is negative, apply negative sign in and outside the square root in equation (35)

Kendall's Tau Correlation Coefficient

Kendall's Tau is a nonparametric measure similar to Spearman rank correlation coefficient, but provides unbiased estimator of the population rank correlation. In this case, the data consists of random sample of n paired numeric or non-numeric observations that are measured on at least ordinal scale.

Computing Kendall's Tau by Neighbors Swaps

This is simple function of the minimum number of neighbor swaps needed to produce one ordering from another. The objects of consideration can be numeric or non-numeric. Considering non-numeric objects, A, B, C, D and the two orderings D, B, A, C and A, B, D, C, the first ordering is converted to into second ordering using neighbor swaps by swapping A and D to get A, B, D, C (Aliyu, 2023). When n items are to be ordered and a minimum of Q swaps is required, the Kendall's denoted by

$$Q = 1 - \frac{4Q}{n(n-1)}, -1 \leq \tau \leq 1,$$

Illustrative Example 1

This method is illustrated with order of performance of numeric data as shown in Table 1:

Table 2: Order of Performance in X and Y

X	5	9	2	6	10	1	4	7	3	8
Y	5	8	1	4	10	2	6	7	3	9

Table 3: Arrangement of X in Order of Magnitude

X	1	2	3	4	5	6	7	8	9	10
Y	2	1	3	6	5	4	7	9	8	10

In order to make Y in the same increasing order as X, swap 2 and 1 to have

Table 4: Output of First Swap

X	1	2	3	4	5	6	7	8	9	10
Y	1	2	3	5	6	4	7	9	8	10

Subsequent swaps are reproduced in Tables 4-6

Table 5: Output of Second Swap

X	1	2	3	4	5	6	7	8	9	10
Y	1	2	3	4	5	6	7	9	8	10

Table 6: Output of Third Swap

X	1	2	3	4	5	6	7	8	9	10
Y	1	2	3	5	4	6	7	9	8	10

Table 7: Output of Fourth Swap

X	1	2	3	4	5	6	7	8	9	10
Y	1	2	3	4	5	6	7	9	8	10

Table 8: Output of Fifth Swap

X	1	2	3	4	5	6	7	8	9	10
Y	1	2	3	4	5	6	7	8	9	10

Thus Q = 5 $\hat{\tau} = 0.78$

Kendall's Tau Correlation by Concordances and Discordances

This is a non-parametric measure with the same assumptions as Spearman's method, but provides unbiased estimator of the population correlation rank. A pair of variable values is said to be concordant if the number of pairs is in natural order. Conversely, A pair of variable values is said to be discordant if the number of pairs is in reverse natural order. KTC|CD is defined as

$$\hat{\tau} = \frac{n_c - n_d}{\frac{1}{2}n(n-1)}$$

n = number of observations, nc = number of concordant pairs and nd = number of discordant pairs

In order to obtain concordant and discordant pairs, the elements of the first quantity X are ranked in ascending order and the concordant and discordant pairs are observed from the elements of the second quantity Y at each point.

Kendall's Tau-b Correlation Coefficient

Kendall's tau b correlation makes adjustment for ties and denoted by

$$\hat{\tau}_B = \frac{n_c - n_d}{\sqrt{(n_0 - n_1)(n_0 - n_2)}}, \quad -1 \leq \hat{\tau}_B \leq 1$$

where

$n =$ Number $n_c =$ of observations, number of concordant pairs, number of discordant pairs

$n_0 = ½ n(n-1)$, $n_1 = \Sigma t_i(t_i-1)/2 = ½[n(n-1)+n(n-1)]$, $n_2 = \Sigma t_j(t_j-1)/2 = ½[n(n-1)+n(n-1)]$

$t_i =$ number of tied observations in the ith group of ties for the first quantity

$t_j =$ number of tied observations in the jth group of ties for the second quantity

Median Correlation Coefficient (MCC)

MCC is a non-parametric measure of a relationship based on median and Median Absolute Deviation (MAD) of two variables x and y and it is denoted by

$$r_{MED} = Median \frac{(x - median(x))}{MAD(x)} \cdot \frac{(y - median(y))}{MAD(y)},$$

Where,

MAD(x) =Median(|x-median(x)|)
Median(x) =Median of x variable
Similarly,
MAD(y) =Median(|y-median(y)|)
Median(y) =Median of y variable. See (Shafiullah & Khau, 2012)

Quadrant Correlation Coefficient (QCC)

Quadrant Correlation Coefficient is a measure that makes use of sign function rather than the rank of observations. It is defined as

$$r_Q = \frac{\sum sign(x_i - Median(x))sign(y_i - Median(y))}{n},$$

Contingency Coefficient

This method uses the chi-squared statistic and the grand total to measure the association between two dichotomous variables. It is given by

$$\emptyset' = \sqrt{\frac{\chi^2}{\chi^2+n}}$$

This coefficient does not have desirable characteristic ranging between 0 and 1 and its zero when $\chi^2 = 0$

Phi Correlation Coefficient

The Phi (ϕ) Correlation coefficient is used to measure the correlation between two variables expressed in form of natural dichotomies. It has same relation with Tetrachoric coefficient as Point Biserial has with Biserial correlation coefficient. Phi correlation also has a relationship with χ^2 expressed as $\chi^2 = N\phi^2$ When there is no trust about the exact nature of dichotomized variables, it is used and expressed as

$$\phi = \frac{PS-QR}{\sqrt{(P+R)(Q+S)(P+Q)(R+S)}}$$

where P,Q,R,S represent the frequencies of the cells in the 2x2 table shown:

Table 8: Dichotomous Bivariate Data into a 2 x 2 Contingency for ϕ

	Item X		Total
	P	Q	P+Q
Item Y	R	S	R+S
	P+R	Q+S	P+Q+R+S

This method of coefficient is given by $\phi = \sqrt{\frac{\chi^2}{N}}$ and its value is based on χ^2 that is uncorrelated for continuity using dichotomous bivariate data into a 2 x 2 contingency in Table 8.

Yule's Coefficient

This coefficient proposed by Yule (1950) is given as

$$Q = \frac{O_{11}O_{22} - O_{12}O_{21}}{O_{11}O_{22} + O_{12}O_{21}} = \frac{\frac{(O_{11}O_{22})}{(O_{12}O_{21})} - 1}{\frac{(O_{11}O_{22})}{(O_{12}O_{21})} + 1} = \frac{\hat{\theta} - 1}{\hat{\theta} + 1}$$

where θˆis the odd ratio.

Q_{ij} =+1 or -1 if any of it is zero and Q_{ij} is undefined if the two entries in a row or column are zero. In this case and for a reasonable estimate of Q to be provided, a corrected estimate of Q is used as

$$\tilde{Q} = \frac{\left(O_{11} + \frac{1}{2}\right)\left(O_{22} + \frac{1}{2}\right) - \left(O_{12} + \frac{1}{2}\right)\left(O_{21} + \frac{1}{2}\right)}{\left(O_{11} + \frac{1}{2}\right)\left(O_{22} + \frac{1}{2}\right) + \left(O_{12} + \frac{1}{2}\right)\left(O_{21} + \frac{1}{2}\right)}$$

Biserial Correlation Coefficient (BCC)

BCC measures the strength of relationship between a continuous variable and an artificially dichotomous (a recoded binary) variable based on some criteria or certain threshold. Computing the correlation between intelligent Quotient (IQ) and the score on a certain test will only measure whether the test is passed or failed. For example, during clinical trials, one may desire to obtain the correlation between the age and hypertension status of sampled persons. In this case, their ages are continuously and normally distributed. However, the hypertension status is determined by the threshold of systolic blood pressure (hypertensive or normal).

Assumptions for Biserial Correlation Coefficient

The correlation has continuity in the dichotomized trait
(b) There is normality of the distribution underlying the dichotomy
(c) Biserial correlation gives an estimate of the product moment for any given data
(d) There is a large value of N
(e) The correlation is not limited to a range of ± 1
(f) There is presence of a split near the median

Computation of Biserial Correlation Coefficient

Biserial Correlation is defined by

$$r_{bis=} \frac{\bar{X}_p - \bar{X}_q}{S_X}\left(\frac{pq}{h}\right)$$

The respective means of X individuals in categories 1 and 0 are specified:

$$\bar{X}_p = \frac{1}{n}\sum_{i=1}^{n_p} X_{pi}$$

$$\bar{X}_q = \frac{1}{n_q}\sum_{i=1}^{n_q} X_{qi}$$

The respective proportions of the total sample in categories 1 and 0 are also given as:

$$p = \frac{n_p}{n} \quad \text{and} \quad q = \frac{n_q}{n}$$

The standard deviation of X for the total sample of n individuals is given as:

$$S_X = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2}$$

The number of observations in categories 1 and 2 and their sum are:

$$n_p = np, n_q = nq \; and \; n = n_p + n_q$$

The ordinate (height) of the standard normal distribution at the point of division between the proportion p and q of the curve is defined as

$$h = \frac{1}{\sqrt{2\pi}} e^{\frac{1}{2}u^2}$$

where u is the threshold for the probability from the standard normal distribution defined as

P(Z ≥ u)= p.

Thus,

$\phi(u) = p, \phi(-u) = q \ and \ \phi^{-1}(p) = \phi^{-1}(q) = u$

Remark:

Alternatively, a biserial correlation coefficient can also be computed using $r_{bis=} \frac{\bar{X}_p - \bar{X}_t}{s_X}\left(\frac{p}{h}\right)$, where $\bar{X}_t$is the mean of the entire group in place of $\bar{X}_q$.

Illustrative Example 2

Table 8: Distribution of Achievement Test Scores for Two Groups

Achievement Test Score (ATS)	Passed (x)	Failed (y)
195-204	7	0
185-194	16	0
175-184	10	6
165-174	35	15
155-164	24	40
145-154	15	26
135-144	10	13
125-134	3	5
115-124	0	5

Assigning the values to the variables based on r_{bis} $p = 0.52, q = 0.48 \ and \ h = 0.394$ that Table 9 is generated to facilitate the computation of equations (46) and (47)

Table 9: Distribution of Achievement Test Scores across the Entire Group

								Entire Group	
ATS	Higher Group (x)	Lower Group (y)	x'	fx'	y'	fy'	z'	fz'	fz'^2
195-204	7	0	4	28	4	0	4	28	112
185-194	16	0	3	48	3	0	3	48	144
175-184	10	6	2	20	2	12	2	32	64
165-174	35	15	1	35	1	15	1	50	50
155-164	24	40	0	0	0	0	0	0	0
145-154	15	26	-1	-15	-1	-26	-1	-41	41
135-144	10	13	-2	-20	-2	-26	-2	-46	92
125-134	3	5	-3	-9	-3	-15	-3	-24	72
115-124	0	5	-4	0	-4	-20	-4	-20	80

From Table 9, $n_1 = 120, n_2 = 120, N = 230, \sum fx' = 87,\ \sum fy' = -60,\ \sum fz' = 27,\ \sum fz'^2 = 27,$ $\bar{X}_p = 156.75, \bar{X}_q = 144.05, S_X = 16.83, r_{bis} = 0.47$

Point-Biserial Correlation Coefficient (PBCC)

Point-biserial correlation coefficient, denoted by r_{pbis}, is a special case of the product-moment correlation r between a continuous variable and another naturally dichotomous variable. In order to estimate the relationship between the underlined variables, the appropriate correlation coefficient is point biserial. Suppose we want to find the correlation between a continuous random variable Y and a binary random variable X which takes the values zero and one. Assume that n paired observations (Y_k, X_k), k = 1, 2, …, n are available. If the common product-moment correlation r is computed from these data, the resulting correlation is called the point-biserial correlation (Mohanty & Misra, 2016).

Computation Point-Biserial Correlation Coefficient

Point-Biserial Correlation Coefficient is defined as

$$r_{pbis} = \frac{\bar{X}_p - \bar{X}_q}{S_X}\sqrt{pq}$$

The respective means of X individuals in categories 1 and 0 are given as:

$$\bar{X}_p = \frac{1}{n_p}\sum_{i=1}^{n_p} X_{pi} \text{ and } \bar{X}_q = \frac{1}{n_q}\sum_{i=1}^{n_q} X_{qi}$$

The respective proportions of the total sample in categories 1 and 0 are as specified:

$$p = \frac{n_p}{n} \ and\ q = \frac{n_q}{n}$$

The standard deviation of X for the total sample of n individuals is equation (48).

Assumptions of Point Biserial Correlation

(i) One of the two variables is continuous on a measurement scale.
(ii) There are no outliers for any continuous variable versus the dichotomous variable.
(iii) The continuous variable is normally distributed within each subgroup when sample size is small.
(iv) The continuous variables have equal variances with the dichotomous variables.

Derivation of Point Biserial Correlation

Proof:

The point biserial correlation is derived from the Pearson's Product Moment Correlation Coefficient in equation (12).

Assign 0 on variable Y to all members of category 0 and 1 to all members of category 1.

Let

$$\sum Y = n_p = np$$

$$\sum Y^2 = n_p = np$$

XY = 0 for all members in category 0

$\sum XY = n_p$ =np

Substituting $\sum XY = n_p\bar{X}_p$; $\sum Y = np$; $\sum Y^2 = np$ into equation

$$r_{pb} = \frac{n\left(n_p\bar{X}_p\right) - (\sum X)(np)}{\sqrt{\left[n\sum X^2 - (\sum x)^2\right]\left[n(np) - (n)^2\right]}}$$

Taking $\sum X = n_p\bar{X}_p + n_q\bar{X}_q, p = 1 - q$ and dividing numerator and denominator of equation (12) by n, we have

$$r_{pb} = \frac{\frac{n_p\bar{X}_p}{n} - p\left(\frac{n_p\bar{X}_p}{n} + \frac{n_p\bar{X}_p}{n}\right)}{\sqrt{n\sum X^2 - (\sum X)^2 - p\frac{(1-p)}{n}}}$$

$$= \frac{p\bar{X}_p - p^2\bar{X}_p - pq\bar{X}_q}{S_X\sqrt{\frac{n-1}{n}}\sqrt{pq}}$$

$$= \frac{p(\bar{X}_p(1-p) - q\bar{X}_q}{S_X\sqrt{\frac{n-1}{n}}\sqrt{pq}}$$

$$= \frac{pq(\bar{X}_p - \bar{X}_q)}{S_X\sqrt{\frac{n-1}{n}}\sqrt{pq}}$$

$$= \frac{\bar{X}_p - \bar{X}_q}{S_X}\sqrt{\frac{n}{n-1}}\sqrt{pq} \quad (60)$$

$= \frac{\bar{X}_p - \bar{X}_q}{S_X}\sqrt{pq}$ as n becomes large so that $\sqrt{\frac{n}{n-1}}$ approximates to unity.

Illustrative Example 3

Table 10: Distribution of 100 Students on Tests X as Correct or Wrong (1 and 0)

Score on Test X	Correct Respondents	Wrong Respondents
70-74	3	0
65-69	6	1
60-64	6	2
55-59	5	4
50-54	6	2
45-49	7	6
40-44	6	8
35-39	3	6
30-34	3	9
25-29	1	4
20-24	0	12

Table 11: Spreadsheet for the Computation of Point Biserial Correlation

Scores on Test x	Correct Respondents	Wrong Respondents	x'	fx'	z'	fz'	fz'^2
70-74	3	0	5	15	5	15	75
65-69	6	1	4	24	4	28	112
60-64	6	2	3	18	3	24	72
55-59	5	4	2	10	2	18	36
50-54	6	2	1	6	1	8	8
45-49	7	6	0	0	0	0	0
40-44	6	8	-1	-6	-1	-14	14
35-39	3	6	-2	-6	-2	-18	36
30-34	3	9	-3	-9	-3	-36	108
25-29	1	4	-4	-4	-4	-20	80
20-24	0	12	-5	0	-5	-60	300

$n_1 = 46, n_2 = 54, N = 100, \sum fx' = 48, \sum fz' = 55, \sum fz'^2 = 841,\ p = 0.46,$
$\bar{X}_p = 52.2, \bar{X}_q = 44.2, S_X = 14.23, r_{pbis} = 0.52$

Tetrachoric Correlation Coefficient

Tetrachoric correlation coefficient denoted by r_t is used when two categorized variables are artificially dichotomized. The variables are expected to be continuous, normally distributed and linearly related to each other. For example, in the study of the relationship between intelligence and emotional maturity, the first variable can be dichotomized as “above average” and “below average” and the other variable as emotionally mature and emotionally immature. In order to compute the tetrachoric correlation coefficient between intelligence and emotional maturity, a 2x2 in Table 12 is used:

Table 12: Dichotomous Bivariate Data into a 2 x 2 Contingency for r_t

	Below Average	Above Avearge
Emotional Maturity	P	Q
Emotional Immaturity	R	S

Step 2: Forward Sweep for state variables

Compute while k = 0,1, 2, N do x_i^{i+1} from equations (10) to (17) respectively and sequentially.

Step 3: Backward Sweep for adjoint variables

Set $j = N + 2 - i$ and compute λ_i^{j-1} from equations (22) to (29) respectively *Step 4: Control Characterization* Compute control within bounds $u_r^* = \min\{\max\{u_{min}, u_r, \}, u_{max}\}$ for $r = 1, \cdots, m$ from equation (18)

Step 5: Termination criteria

If termination conditions are met go to step 6 otherwise step 7

Step 6: Output $x^k_i, \lambda^j_i, u^*_i (\forall i,j)$ and end function *Step 7: Return* Repeat step 2

2: Numerical simulations: Implementation and Results

Example 1: Considering the optimal control problem below

$$\text{Min } J[u] = \min\int_0^1 u(t)2\,dt,$$

$$x'(t) = x(t) + u(t), \quad (30)$$

$$x(0) = 1,\ x(1) \text{ free.}$$

The Hamiltonian function H is defined as $H = u(t)^2 + \lambda(t)\cdot(x(t)+u(t))$ where $\lambda(t)$ is the adjoint variable (or costate). Using the optimality adjoint and transversality conditions yields the analytical (exact) optimal solution below:

$$x^*(t) = e^t, \qquad u^*(t) = 0. \quad (31)$$

The optimal control obtained using the optimality condition, $\frac{\partial H}{\partial u} = 0$, is given by

$$\begin{aligned} u^*(t) &= -\frac{\lambda(t)}{2}, \\ &= \min\left(u_{\max},\ \max\left(u_{min}, -\frac{\lambda(t)}{2}\right)\right) \end{aligned} \quad (32)$$

ascertained to be minimum since $\frac{\partial^2 H}{\partial u^2} = 2 > 0.$

The derived costate equation using the adjoint conditions, $\lambda'(t) = -\frac{\partial H}{\partial I(t)}$, given by:

$$\lambda'(t) = -\lambda(t), \quad \lambda(T) = 0 \quad (33)$$

Applying the forward Euler, RK4 and the proposed RK6 forward -backward sweep methods (i.e RK4FBSM and proposed RK6FBSM respectively) yields the results below.

Table1: Result of State variable for example 1

S/N	Exact	Euler		RK4FBSM		Proposed RK6FBSM	
	x_A	x_E	$\|x_A - x_E\|$	$xK4$	$\|xA - xK4\|$	$xK6$	$\|xA - xK6\|$
1	1.1051709181	1.1111111111	5.9401930000 $\times10^{-3}$	1.1051708333	8.47000 $\times10^{-8}$	1.1051709181	0.00000 $\times 10^0$
2	1.2214027582	1.2345679012	1.3165143100 $\times10^{-2}$	1.2214025709	1.87300 $\times10^{-7}$	1.2214027582	0.00000 $\times10^0$
3	1.3498588076	1.3717421125	2.1883304900 $\times10^{-2}$	1.3498584971	3.10500$\times10^{-7}$	1.3498588076	0.00000 $\times10^0$
4	1.4918246976	1.5241579028	3.2333205100 $\times10^{-2}$	1.4918242401	4.57600 $\times10^{-7}$	1.4918246977	0.00000 $\times10^0$

5	1.6487212707	1.6935087808	4.4787510100 $\times10^{-2}$	1.6487206386	6.32100 $\times10^{-7}$	1.6487212707	0.00000 $\times10^{0}$
6	1.8221188004	1.8816764232	5.9557622800 $\times10^{-2}$	1.8221179621	8.38300 $\times10^{-7}$	1.8221188004	0.00000 $\times10^{0}$
7	2.0137527075	2.0907515813	7.6998873800 $\times10^{-2}$	2.0137516266	1.08090 $\times10^{-6}$	2.0137527075	0.00000 $\times10^{0}$
8	2.2255409285	2.3230573125	9.7516384100 $\times10^{-2}$	2.2255395633	1.36520 $\times10^{-6}$	2.2255409285	0.00000 $\times10^{0}$
9	2.4596031112	2.5811747917	1.2157168060 $\times10^{-1}$	2.4596014138	1.69740 $\times10^{-6}$	2.4596031112	0.00000 $\times10^{0}$
10	2.7182818285	2.8679719908	1.4969016230$\times10^{-1}$	2.7182797441	2.08430$\times10^{-6}$	2.7182818285	0.00000 $\times10^{0}$

Table 1: $|x_A - x_E|$, $|x_A - x_{K4}|$and$|x_A - x_{K6}|$ ≡ errors of Euler RK4 & RK6 respectively

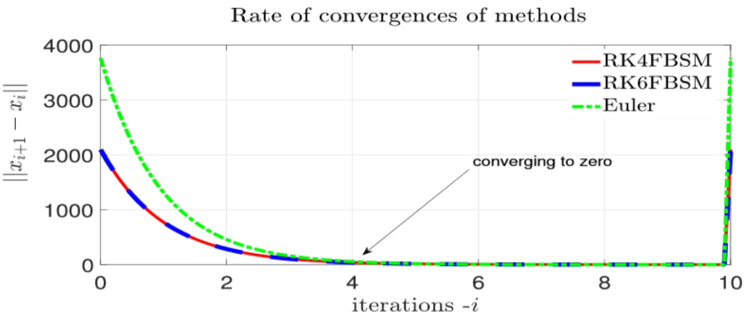


Figure 1: Rate of convergence in 10 iters.

Example 2: Considering the SIS Model with Treatment [9]

$$\min C[u] = \int_0^T \omega_1 I(t) + u^2(t))\, dt,$$
$$s.t : \dot{I}(t) = \beta \ (N - I(t))I(t) - (\mu+\gamma)I(t) - u(t)I(t) \quad (34)$$

(35)

$$I(0) = I_0, I(T) free. \quad (36)$$

The Hamiltonian is given by:

$H(I(t),u(t),\lambda(t)) = \omega_1 I(t) + u^2(t) + \lambda(t)(\beta(N - I(t))I(t) - (\mu+\gamma)I(t) - u(t)I(t)$(37) The optimal control obtained using the optimality condition, $\frac{\partial H}{\partial u}= 0$, is given by

$$u^*(t) = \frac{\lambda(t)I(t)}{2},$$
$$= \min\left(u_{\max}, \max\left(u_{min}, \frac{\lambda(t)I(t)}{2}\right)\right). \quad (38)$$

ascertained to be minimum since $\frac{\partial^2 H}{\partial u^2} = 2 > 0.$

The derived co-state equation using the adjoint conditions, $\lambda'(t) = -\frac{\partial H}{\partial I(t)}$, given by:

$\lambda'(t) = -\omega_1 - \lambda(t)\beta\,(N - I(t)) - \beta I(t) - (\mu + \gamma) - u(t),\ \lambda(T) = 0$ (39)

Applying the forward Euler, RK4 and the proposed RK6 forward -backward sweep methods (i.e. RK4FBSM and proposed RK6FBSM respectively) also yields the results in Table 2 below using the following parameters: $\beta = 0.05$, $\mu = 0.01$, $\gamma = 0.5$, $N = 100$, $\omega_1 = 1$ and $T = 1$.

Table 2: Result of State and Control variables for example 2

S/N	Euler		convergence		Proposed RK6FBSM	
	x_E	u_E	$xK4$	$uK4$	$xK6$	$uK6$
1	10.0000000000	5.2355651638	10.0000000000	4.5926947060	10.0000000000	4.6363573386
2	8.7650656568	4.6326137300	9.5613737942	4.3167361686	9.5464589222	4.3768363778
3	8.2556597311	4.1600567381	9.4089685710	4.0418362859	9.3440040276	4.1061078144
4	8.1851105244	3.7431700492	9.5201882548	3.7594888052	9.3763319652	3.8164326820
5	8.4592147545	3.3460084781	9.9038244602	3.4602903181	9.6519009702	3.4992076079
6	9.0673116818	2.9449889133	10.6018768364	3.1325900058	10.2060033528	3.1440596831
7	10.0557266500	2.5197980734	11.7007294372	2.7604692418	11.1093962855	2.7374992954
8	11.5303031948	2.0484433716	13.3574883436	2.3201655255	12.4871637697	2.2605946027
9	13.6800933636	1.5026879752	15.8577984930	1.7728678617	14.5571182701	1.6844954512
10	16.8306930352	0.8415968385	19.7510850824	1.0482398348	17.7109254612	0.9609642283
11	21.5547425985	0.0000000000	26.2132226347	0.0000000000	22.7016008493	0.0000000000

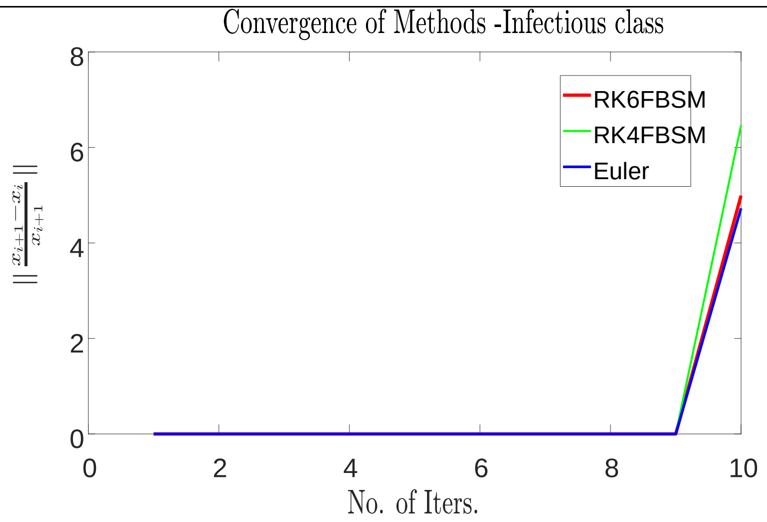


Figure 2: Rate of convergence in 10 iterations.

Example 3: We considered the model on optimal control and comprehensive cost effectiveness analysis for COVID-19 [2]

$$J(u_1,u_2,u_3,u_4) := \min \int_0^T \left[A_1E + A_2I + A_3A + A_4B + \frac{1}{2}\sum_{i=1}^{4} D_i u_i^2(t)\right] dt \tag{40}$$

Subject to the non-autonomous system below

$$\begin{cases} \frac{dS}{dt} &= \Lambda - (1-u_1(t))\left(\frac{\beta_1 E+\beta_2 I+\beta_3 A}{N}\right) S - (1-u_1(t)-u_2(t))\beta_4\frac{B}{N}S - dS, \\ \frac{dE}{dt} &= (1-u_1(t))\left(\frac{\beta_1 E+\beta_2 I+\beta_3 A}{N}\right) S + (1-u_1(t)-u_2(t))\beta_4\frac{B}{N}S - (\delta+d)E, \\ \frac{dI}{dt} &= (1-\tau)\delta E - (d+d_1+\gamma_1)I, \\ \frac{dA}{dt} &= \tau\delta E - (d+\gamma_2)A, \\ \frac{dR}{dt} &= \gamma_1 I + \gamma_2 A - dR, \\ \frac{dB}{dt} &= (1-u_3(t))(\psi_1 E + \psi_2 I + \psi_3 A) - (u_4(t)+\phi)B, \end{cases} \tag{41}$$

where $A_i > 0 (i = 1,2,3,4)$. The derived adjoint equations were

$$\begin{cases} \frac{d\lambda_1}{dt} = (\lambda_1-\lambda_2)((1-u_1)\left(\frac{\beta_1 E^*+\beta_2 I^*+\beta_3 A^*}{N^2}\right)(E^*+I^*+A^*+R^*))+ \\ (\lambda_1-\lambda_2)(1-u_1-u_2)\beta_4\frac{B^*}{N^2}(E^*+I^*+A^*+R^*)+\lambda_1 d, \\ \frac{d\lambda_2}{dt} = -A_1 + (\lambda_1-\lambda_2)(1-u_1)S^*\left(\frac{(S^*+I^*+A^*+R^*)\beta_1-(\beta_2 I^*+\beta_3 A^*)}{N^2}\right)+ \\ (\lambda_2-\lambda_1)(1-u_1-u_2)\beta_4\frac{B^*S^*}{N^2} + (\delta+d)\lambda_2 - \lambda_2(1-\tau)\delta\lambda_3 - \tau\delta\lambda_4 - (1-u_3)\psi_1\lambda_6 \\ \frac{d\lambda_3}{dt} = -A_2 + (\lambda_1-\lambda_2)(1-u_1)S^*\left(\frac{(S^*+E^*+A^*+R^*)\beta_2-(\beta_1 E^*+\beta_3 A^*)}{N^2}\right)+ \\ (\lambda_2-\lambda_1)(1-u_1-u_2)\beta_4\frac{B^*S^*}{N^2} + (\delta+d_1+\gamma_1)\lambda_3 - \gamma_1\lambda_5 - (1-u_3)\psi_2\lambda_6, \\ \frac{d\lambda_4}{dt} = -A_3 + (\lambda_1-\lambda_2)(1-u_1)S^*\left(\frac{(S^*+E^*+I^*+R^*)\beta_3-(\beta_1 E^*+\beta_2 I^*)}{N^2}\right)+ \\ (\lambda_2-\lambda_1)(1-u_1-u_2)\beta_4\frac{B^*S^*}{N^2} + (d_1+\gamma_2)\lambda_4 - \gamma_2\lambda_5 - (1-u_3)\psi_3\lambda_6, \\ \frac{d\lambda_5}{dt} = (\lambda_2-\lambda_1)(1-u_1)\left(\frac{(\beta_1 E^*+\beta_2 I^*+\beta_3 A^*)S^*}{N^2}\right)+ \\ (\lambda_2-\lambda_1)(1-u_1-u_2)\beta_4\frac{S^*}{N^2} + \lambda_5 d, \\ \frac{d\lambda_6}{dt} = -A_4 + (\lambda_1-\lambda_2)(1-u_1-u_2)\beta_4\frac{S^*}{N} + (u_4+\phi)\lambda_6 d, \end{cases} \tag{42}$$

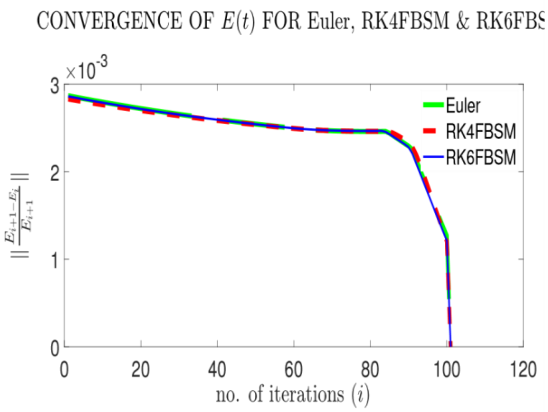
while the optimal control characterizations were;

$$u_1^*(t) = \min\left\{\max\left\{0, \frac{(\lambda_2-\lambda_1)(\beta_1 E^* + \beta_2 I^* + \beta_3 A^* + \beta_4 B^*)S}{D_1 N}\right\}, u_{1\max}\right\}$$
$$u_2^*(t) = \min\left\{\max\left\{0, \frac{(\lambda_2-\lambda_1)\beta_4 B^* S^*}{D_2 N}\right\}, u_{2\max}\right\},$$
$$u_3^*(t) = \min\left\{\max\left\{0, \frac{\lambda_6(\psi_1 E^* + \psi_2 I^* + \psi_3 A^*)}{D_3}\right\}, u_{3\max}\right\},$$
$$u_4^*(t) = \min\left\{\max\left\{0, \frac{\phi B^* \lambda_6}{D_4}\right\}, u_{4\max}\right\}. \quad (43)$$

Simulating with the following parameters $\beta_1 = 0.1233$; $\beta_2 = 0.0542$; $\beta_3 = 0.0020$; $\beta_4 = 0.1101$; $\delta = 0.1980$; $\tau = 0.3085$; $d = 1/(74.87 * 365)$; $d_1 = 0.0104$; $\gamma_1 = 0.3680$; $\gamma_2 = 0$; $\psi_1 = 0.2574$; $\psi_2 = 0.2798$; $\psi_3 = 0.1584$; $\phi = 0.3820$ yields the results below.

Table 3: Convergence analysis of State variable ($E(t)$) for example 3

S/N	Euler		RK4FBSM		Proposed RK6FBSM	
	E_E	$\left\lVert\frac{E_{i+1}-E_i}{E_{i+1}}\right\rVert$	$EK4$	$\left\lVert\frac{E_{i+1}-E_i}{E_{i+1}}\right\rVert$	$EK6$	$\left\lVert\frac{E_{i+1}-E_i}{E_{i+1}}\right\rVert$
1	1.5000000000	-	1.5000000000		1.5000000000	
11	1.4586854415	2.7646377×10^{-3}	1.4582818367	2.7890189×10^{-3}	1.4581829510	2.7953366×10^{-3}
21	1.4194850125	2.6987961×10^{-3}	1.4187988721	2.7167244×10^{-3}	1.4186243717	2.7216273×10^{-3}
31	1.3821955578	2.6394372×10^{-3}	1.3813219909	2.6520393×10^{-3}	1.3810945185	2.6556630×10^{-3}
41	1.3466385402	2.5859736×10^{-3}	1.3456514066	2.5942269×10^{-3}	1.3453892655	2.5968128×10^{-3}
51	1.3126570130	2.5378496×10^{-3}	1.3116129021	2.5425930×10^{-3}	1.3113294894	2.5443931×10^{-3}
61	1.2801128162	2.4946384×10^{-3}	1.2790541427	2.4967666×10^{-3}	1.2787595421	2.4977039×10^{-3}
71	1.2488168407	2.4685349×10^{-3}	1.2477535795	2.4713852×10^{-3}	1.2474913995	2.4675198×10^{-3}
81	1.2184644912	2.4616005×10^{-3}	1.2173844274	2.4656931×10^{-3}	1.2171894367	2.4600497×10^{-3}
91	1.1893046217	2.3341404×10^{-3}	1.1885613052	2.2797627×10^{-3}	1.1883097475	2.2930852×10^{-3}
101	1.1685184378	1.2045593×10^{-3}	1.1684734094	1.2114794×10^{-3}	1.1676305020	1.2714446×10^{-3}



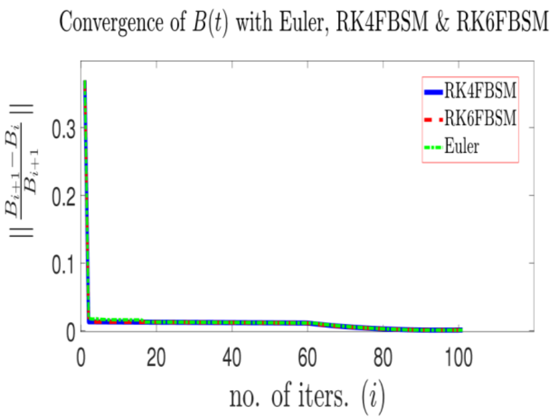


Fig. 3: Convergence of $E(t)$ in 101 iterations. Fig 4: Convergence of $B(t)$ in 101 iterations.

DISCUSSION OF RESULTS

In example 1, the rate of convergence of the 3 methods: Euler, RK4 and Rk6 were compared on the state variable as demonstrated on table 1. It was discovered that the rate of convergence of the RK6 compares favorably with RK4 with higher level of accuracy after 10 iterations. In similar manner, Table 2 and 3 were used to compare the Iterates for the Euler, RK4 and RK6 forward-backward sweep methods on the state variables of examples 2 and 3 respectively. Figures 2, 3 and 4 were used to illustrate the rate of convergences which shows that the RK6FBSM performs excellently well although the computational efforts is more in terms of rigors of coding and process time.

CONCLUSION

The adaptation of the 6th order Runge-Kutta forward-backward sweep algorithm for solving generalized optimal control problems with bounded control arrives at an accurate result at a faster rate of convergence compared to the Runge-Kutta of order four (RK4), due to its stability and higher numerical order of convergence. This adaptation is essential for handling mathematical models with large number of non-linear dynamical equations. Therefore, the sixth order Runge-Kutta forward-backward sweep algorithm seeks to provide a more effective and efficient method due to its speed, accuracy, higher rate of convergence, suitability and versatility for real-time or practical applications such as the Epidemiological and general Biomedical models (see MATLAB code in Appendix).

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