

Approximation of Iteration Number for Gauss-Seidel Using Redlich-Kister Polynomial

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Abstract: Problem statement: Development of mathematical models based on set of observed data plays a crucial role to describe and predict any phenomena in science, engineering and economics. Therefore, the main purpose of this study was to compare the efficiency of Arithmetic Mean (AM), Geometric Mean (GM) and Explicit Group (EG) iterative methods to solve system of linear equations via estimation of unknown parameters in linear models. **Approach:** The system of linear equations for linear models generated by using least square method based on $(m+1)$ set of observed data for number of Gauss-Seidel iteration from various grid sizes. Actually there were two types of linear models considered such as piece-wise linear polynomial and piece-wise Redlich-Kister polynomial. All unknown parameters of these models estimated and calculated by using three proposed iterative methods. **Results:** Thorough several implementations of numerical experiments, the accuracy for formulations of two proposed models had shown that the use of the third-order Redlich-Kister polynomial has high accuracy compared to linear polynomial case. **Conclusion:** The efficiency of AM and GM iterative methods based on the Redlich-Kister polynomial is superior as compared to EG iterative method.

Key words: Arithmetic mean, geometric mean, explicit group, Redlich-Kister model, Poisson equation

INTRODUCTION

Group Explicit iterative method has been formulated and proposed by Evans (1985). Further investigation and implementation of this method are done by Evans and Yousif (1986; 1990); Yousif and Evans (1986; 1998) and Jumat and Abdullah (2001). The method is then modified by Abdullah (1991) using half-sweep concept and produced Explicit Decoupled Group (EDG) method. The EDG methods have been further implemented by Ibrahim and Abdullah (1995); Yousif and Evans (1995), Jumat and Abdullah (1999) and Sulaiman *et al.* (2007). Beside that, Othman and Abdullah (2000a; 2000b) proposed a new variant of EG method called the Modified Explicit Group (MEG).

This method implements the quarter-sweep concept to the EG method.

Arithmetic Mean (AM) and Geometric Mean (GM) schemes are methods that are categorized in two-step iterative type. From its literature, Ruggiero and Galligani (1990) is the first to propose the AM method. This method has the same computational molecule to Iterative Alternating Decomposition Explicit (IADE) proposed by Sahimi and Khatim (2001) but different in their parameter coefficient. However, the implementation of the first step formulation and second step formulation is absolutely different.

Sulaiman *et al.* (2004) combined the AM method with the half-sweep concept to develop the Half-Sweep Arithmetic Mean (HSAM). Further investigation to this

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method can be found in Sulaiman *et al.* (2005a; 2005b). In fact, Geometric Mean (GM) method is another alternative to AM method. Sulaiman *et al.* (2006) also proposed the Half-Sweep Geometric Mean (HSGM) to solve two point boundary value problems. The method is further investigated by Abdullah *et al.* (2006) to solve water quality model and Muthuvalu and Sulaiman (2008) for solving linear Fredholm Equations.

In this study, we will implement the EG, AM and GM methods to estimate the unknown parameters via solving system of linear equations. The system of linear equations is generated using the least square method on (m+1) set of observed data. Here, only two types of linear models will be considered, which are the piece-wise linear polynomial (Linear) and piece-wise Redlich-Kister polynomial (RK).

MATERIALS AND METHODS

Generating system of linear equations: To generate the system of linear equations, consider (m+1) data set produced via simulation given in Table 1.

As mentioned before, in this study we only consider the piece-wise linear polynomial and Redlich-Kister polynomial. The piece-wise linear polynomial and the third-order piece-wise Redlich-Kister polynomial are given respectively as follows:

$$y_{1k}(X) = S_{2k-1} + S_{2k}X + e_k, \quad X \in [X_k, X_{k+1}] \tag{1}$$

and:

$$y_{3k}(X) = X(1-X)(S_{2k-1} + S_{2k}(2X-1)) + e_k, \tag{2}$$

$$X \in [X_k, X_{k+1}]$$

Where:

- X_k = k^{th} matrix size
- Y_k = GS number of iterations for k^{th} matrix size
- e_k = k^{th} random error

for $k = 1, 2, 3, \dots, m, m+1$ and S_i $i = 1, 2, 3, \dots, (n = 2m)$, are the unknown parameters which will be estimated. To generate the system of linear equation from observed data, (X_k, Y_k) , $i = 1, 2, 3, \dots, m, m+1$, both Eq. 1 and 2 can be rewritten as:

$$y_k(X) = N_1^k(X)S_{2k-1} + N_2^k(X)S_{2k} + e_k, \tag{3}$$

$$X \in [X_k, X_{k+1}]$$

Meanwhile, the function $N_t^k(x), t=1, 2$ for both Model 1 and 2 are given as follows:

$$\left. \begin{aligned} N_1^k(X) &= 1, \\ N_2^k(X) &= X, \end{aligned} \right\} \quad X \in [X_k, X_{k+1}] \tag{4}$$

Table 1: Relation between matrix size and number of iterations for Gauss-Seidel to solve one dimensional Poisson problem

K	Matrix size	No. of Iterations
1	X_1	Y_1
2	X_2	Y_2
3	X_3	Y_3
\vdots	\vdots	\vdots
m	X_m	Y_m
m+1	X_{m+1}	Y_{m+1}

and

$$\left. \begin{aligned} N_1^k(X) &= X - X^2, \\ N_2^k(X) &= 3X^2 - X - 2X^3, \end{aligned} \right\} \quad X \in [X_k, X_{k+1}] \tag{5}$$

Assuming that values between data interval are equal, thus:

$$Y_{k-1}(X_k) \approx N_1^{k-1}(X_k)S_{2k-1} + N_2^{k-1}(X_k)S_{2k}, \tag{6}$$

$$X_k \in [X_{k-1}, X_k]$$

$$Y_k(X_k) \approx N_1^k(X_k)S_{2k-1} + N_2^k(X_k)S_{2k}, \tag{7}$$

$$X \in [X_k, X_{k+1}]$$

The random error $e_k, k = 1, 2, 3, \dots, m, m+1$ can be defined as follows:

$$e_k = \begin{cases} Y_1 - N_{1,1}^1 S_1 - N_{2,1}^1 S_2, & k = 1 \\ Y_{m+1} - N_{1,m+1}^m S_{2m-1} - N_{2,m+1}^m S_{2m}, & k = m + 1 \\ Y_k - N_{1,k}^{k-1} S_{2k-3} - N_{2,k}^{k-1} S_{2k-2} - N_{2,k}^k S_{2k-1} - N_{2,k}^k S_{2k}, & k \neq 1, m + 1 \end{cases} \tag{8}$$

where, $N_t^k(X_p), t, p = 1, 2$ is denoted as $N_{t,p}^k$. Next, we estimate the S_i $i = 1, 2, 3, \dots, (n = 2m)$, which minimized:

$$H = \sum_{k=1}^{m+1} e_k^2 \tag{9}$$

Thus, Eq. 9 has to satisfy Eq. 10:

$$\frac{\partial H}{\partial S_i}, i = 1, 2, 3, \dots, 2m, \tag{10}$$

Eq. 10 will be used to generate system of linear equation in the form of matrix. The general form of generated matrix for the case of $m = 10$ is given by:

$$RS = F \tag{11}$$

Where:

$$R = \begin{bmatrix} R_{1,1} & R_{1,2} & R_{1,3} & R_{1,4} & & & & & & & \\ R_{2,1} & R_{2,2} & R_{2,3} & R_{2,4} & & & & & & & \\ R_{3,1} & R_{3,2} & R_{3,3} & R_{3,4} & R_{3,5} & R_{3,6} & & & & & \\ R_{4,1} & R_{4,2} & R_{4,3} & R_{4,4} & R_{4,5} & R_{4,6} & & & & & \\ & & R_{5,3} & R_{5,4} & R_{5,5} & R_{5,6} & R_{5,7} & R_{5,8} & & & \\ & & R_{6,3} & R_{6,4} & R_{6,5} & R_{6,6} & R_{6,7} & R_{6,8} & & & \\ & & & & R_{7,5} & R_{7,6} & R_{7,7} & R_{7,8} & R_{7,9} & R_{7,10} & \\ & & & & R_{8,5} & R_{8,6} & R_{8,7} & R_{8,8} & R_{8,9} & R_{8,10} & \\ & & & & & & R_{9,7} & R_{9,8} & R_{9,9} & R_{9,10} & \\ & & & & & & R_{10,7} & R_{10,8} & R_{10,9} & R_{10,10} & \end{bmatrix}_{(10 \times 10)}$$

$$\underline{S} = [S_1 \ S_2 \ S_3 \ S_4 \ S_5 \ S_6 \ S_7 \ S_8 \ S_9 \ S_{10}]^T \quad (R_{i-1,i-1})(R_{i,i}) - (R_{i,i-1})(R_{i-1,i}) \approx 0 \quad (17)$$

$$\underline{F} = [F_1 \ F_2 \ F_3 \ F_4 \ F_5 \ F_6 \ F_7 \ F_8 \ F_9 \ F_{10}]^T$$

Therefore, we rewrite the system of linear Eq. 15 as:

Referring to the system of linear Eq. 11, the two point EG scheme can be rewritten as (Evans and Yousif, 1986; Jumat and Abdullah, 2001):

$$\begin{bmatrix} \alpha & 1 \\ \beta & 1 \end{bmatrix} \begin{bmatrix} S_{i-1} \\ S_i \end{bmatrix} = \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix} \quad (18)$$

$$\begin{bmatrix} R_{i-1,i-1} & R_{i-1,i} \\ R_{i,i-1} & R_{i,i} \end{bmatrix} \begin{bmatrix} S_{i-1} \\ S_i \end{bmatrix} = \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} \quad (15)$$

Where:

$$\begin{aligned} \alpha &= \frac{R_{i-1,i-1}}{R_{i-1,i}} > 1 \\ \beta &= \frac{R_{i,i-1}}{R_{i,i}} < 1 \\ \rho_1 &= \frac{P_1}{R_{i-1,i}} \\ \rho_2 &= \frac{P_2}{R_{i,i}} \end{aligned}$$

Where:

$$P_1 = \begin{cases} F_1 - R_{1,3}S_3 - R_{1,4}S_4, & i=1 \\ F_{n-1} - R_{n-1,n-3}S_{n-3} - R_{n-1,n-2}S_{n-2}, & i=n-1 \\ F_{i-1} - R_{i-1,i-3}S_{i-3} - R_{i-1,i-2}S_{i-2} - R_{i-1,i+1}S_{i+1} - R_{i-1,i+2}S_{i+2}, & i=3,5,7,\dots,n-3 \end{cases}$$

$$P_2 = \begin{cases} F_2 - R_{2,3}S_3 - R_{2,4}S_4, & i=2 \\ F_n - R_{n,n-3}S_{n-3} - R_{n,n-2}S_{n-2}, & i=n=2m \\ F_i - R_{i,i-3}S_{i-3} - R_{i,i-2}S_{i-2} - R_{i,i+1}S_{i+1} - R_{i,i+2}S_{i+2}, & i=4,6,8,\dots,n-2 \end{cases}$$

Using the Gauss elimination technique to Eq. 18, it can be shown that the coefficient matrix can be rewritten in the form of triangular matrix as:

Using the matrix approach, Eq. 15 can be rewritten as:

$$\begin{bmatrix} 1 & 0 \\ -\beta & 1 \end{bmatrix} \begin{bmatrix} \alpha & 1 \\ \beta & 1 \end{bmatrix} \begin{bmatrix} S_{i-1} \\ S_i \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -\beta & 1 \end{bmatrix} \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix} \quad (19)$$

$$\begin{bmatrix} \alpha & 1 \\ 0 & 1 - \frac{\beta}{\alpha} \end{bmatrix} \begin{bmatrix} S_{i-1} \\ S_i \end{bmatrix} = \begin{bmatrix} \rho_1 \\ \rho_2 - \frac{\beta}{\alpha}\rho_1 \end{bmatrix}$$

$$\begin{bmatrix} S_{i-1} \\ S_i \end{bmatrix} = \frac{1}{(R_{i-1,i-1})(R_{i,i}) - (R_{i,i-1})(R_{i-1,i})} \begin{bmatrix} R_{i,i} & -R_{i-1,i} \\ -R_{i,i-1} & R_{i-1,i-1} \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} \quad (16)$$

Manipulating both Eq. 19, it can be shown that the two point EG scheme with parameter w (denoted as 2 point-EG (SOR)) at (k+1)th iteration as:

However, the two point EG scheme in Eq. 16 still cannot be implemented using computer program since the determinant value is too small relatively, i.e.:

$$\begin{bmatrix} S_{i-1} \\ S_i \end{bmatrix}^{(k+1)} = (1-w) \begin{bmatrix} S_{i-1} \\ S_i \end{bmatrix}^{(k)} + \frac{w}{\alpha-1} \begin{bmatrix} \rho_1 - \rho_2 \\ \alpha\rho_2 - \rho_1 \end{bmatrix}, \quad \alpha > 1 \quad (20)$$

with $1 \leq w < 2$. The implementation of 2 point- EG (SOR) is displayed in Algorithm 2.

Algorithm 2: 2 point-EG (SOR) scheme:

- a. Initialize parameter
 $R, F, S_i^{(0)}, w, EPS_c \leftarrow 5.0E-6$
- b. For $k = 1, 2, 3, \dots, m$, calculate
 - i. Assign ρ_1, ρ_2

$$S_{2k-1}^{(k+1)} \leftarrow (1-w)S_{2k-1}^{(k)} + \left(\frac{w}{\alpha-1}\right)(\rho_1 - \rho_2)$$
 - ii. Calculate

$$S_{2k}^{(k+1)} \leftarrow (1-w)S_{2k}^{(k)} + \left(\frac{w}{\alpha-1}\right)(\alpha\rho_2 - \rho_1)$$
- c. Test convergence for $r \ i = 1, 2, \dots, n$, calculate $|S_i^{(k+1)} - S_i^{(k)}| < EPS$
- d. Repeat b if convergence test is not satisfied

In this research, Gauss-Seidel (GS) iterative scheme will be used as the control of comparison.

RESULTS AND DISCUSSION

Numerical experiment: In this research, we analyze the accuracy of the approximation via both piece-wise polynomial models of Eq. 1 and 2 and compare with the observed data. Furthermore, some numerical experiments have been done to show the performance of AM, GM and EG methods to calculate the S_i for $i = 1, 2, 3, \dots, (n = 2m)$. Results of the numerical experiments for number of iterations, computation time and percentage of average error are given in Fig. 1-3.

Generally, in this research, we use the tolerance error, $\epsilon = 5 \times 10^{-6}$. In the result, we use GS-Linear, AM-Linear, GM-Linear, 2EG(SOR)-Linear, GS-RK, AM-RK, GM-RK and 2EG(SOR)-RK notation to represent the Gauss-Seidel using piece-wise linear polynomial, Arithmetic mean using piece-wise linear polynomial, Geometric mean using piece-wise linear polynomial, 2 point EG(SOR) using piece-wise linear polynomial, Gauss-Seidel using Piece-wise Redlich-Kister polynomial, Arithmetic mean using Piece-wise Redlich-Kister polynomial, Geometric mean using Piece-wise Redlich-Kister polynomial and 2 point EG(SOR) using Piece-wise Redlich-Kister polynomial, respectively.

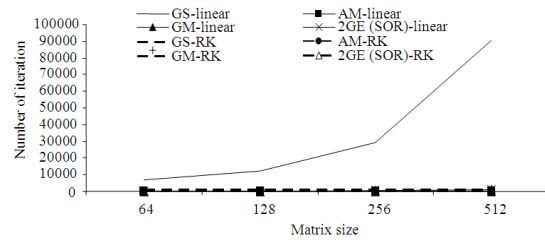


Fig. 1: Comparison of iteration number for all method

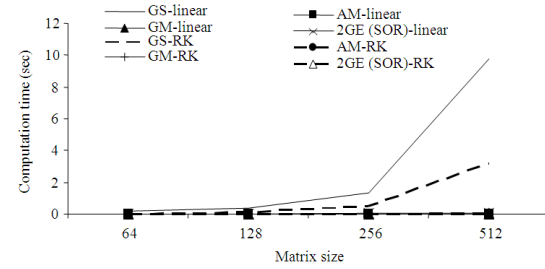


Fig. 2: Comparison of computational time for all method

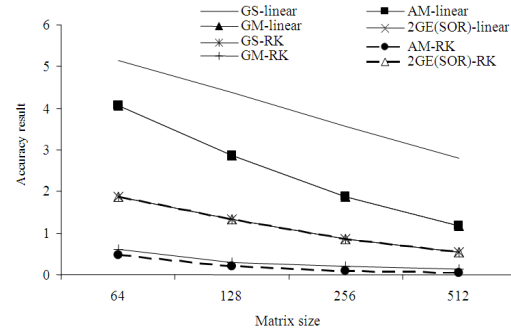


Fig. 3: Percentage of relative average error comparison between methods

CONCLUSION

In this research, formulation of polynomial model for Eq. 1 and 2 can be represented as Eq. 3. Using polynomial in Eq. 3, the system of linear equations generated for both polynomial models can be shown. However, the condition of the coefficient matrix of Eq. 11 is ill (Chiam and Majid, 1990). Therefore, the convergence criteria may not be satisfied. Furthermore, the coefficient matrix is not categorized as positive definite matrix. Thus, a modification has been proposed via Gauss elimination approach.

From the numerical experiment results, Fig. 1 clearly shows that number of iterations for 2 point EG(SOR)-Linear and 2 point EG(SOR)-RK reduce around 98.12-98.39% and 98.22-99.07%, respectively, when compared to GS-Linear. While computational

time in Fig. 2 for both 2 point EG (SOR) schemes reduce around 88.23-99.28% and 94.87-100%. Accuracy results in Fig. 3 show the use of piece-wise third order Redlich-Kister polynomial has high accuracy compared to only using linear polynomial.

Both AM and GM schemes also show tremendous results compared to GS schemes. Figure 1 shows that 99.88-99.97% reduction in number of iterations for AM-Linear and GM-Linear compared to GS-Linear, 77.15-92.57% reduction in number of iterations for AM-RK and 89.31-92.83% reduction for GM-RK. Both AM and GM schemes computational time are almost 100% faster than both GS schemes (Fig. 2). Accuracy results for AM and GM Redlich-Kister scheme are far better than linear polynomial schemes as shown in Fig. 3.

Our next research will be implementing half-sweep (Abdullah, 1991; Ibrahim and Abdullah, 1995), quarter-sweep (Othman and Abdullah, 2000a; 2000b) concept and multigrid (Hackbusch, 1983; Othman and Abdullah, 1999) to solve the same problem.

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