Analysis of Crout, LU, Cholesky Decomposition, and QR Factorization: A Case Study on The Relationship Between Abiotic (Carbon and Nitrogen) and Biotic (Macrobenthos Diversity) Factors

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Abstract - Many real world problems can be represented by a system of linear equations, such as in the field of ecology, i.e. the relationship of carbon and nitrogen with macrobenthos diversity. There are many methods to solve linear equations systems, then it is necessary to do an analysis of which method is the best so that the user can choose the most efficient method. The methods that will be analyzed are LU, Crout, Cholesky decomposition, and QR factorization. From the calculation of arithmetic operations obtained Cholesky decomposition method is the most efficient method because it has the fewest arithmetic operations. Further, to verify the proposed method we demonstrated simulation with a case study of the relationship between carbon and nitrogen with the macrobenthos diversity based on data from the area of polyculture system and PT. Kayu Lapis Indonesia coastal, Mororejo village subdistrict Kaliwungu district Kendal. From the simulation results obtained that computing time the smallest is the Cholesky decomposition is equal to 1.4664 seconds, which means that the Cholesky decomposition is the most efficient method than the method of LU, Crout decomposition and QR factorization.

Keywords — LU Decomposition, Crout decomposition, QR factorization, Cholesky decomposition, Carbon, Nitrogen, Macrobenthos

I. INTRODUCTION

In this research will be presented mathematically relationship between carbon and nitrogen with macrobenthos diversity through regression models, especially on how to determine the parameters of the multiple linear regression equation. In the process of determining the regression parameter is used least squares method that produces systems of linear equations. Here will be studied how to determine the solutions of the system of linear equations. The system of linear equations can be solved by several methods, such as, the LU decomposition method (Chinchole and Bhadane, 2014), Crout decomposition (Supriyono and Daniel, 2005), QR factorization (Bojanczyk, et al., 1986; Rorres, 2004), and Cholesky Decomposition (Robert and Elizabeth, 1990). Therefore, the assessment needs to be conducted to determine the most efficient method.

One of the applications of mathematics in the field of ecology, in this case represents the relationship between organic matter, carbon and nitrogen to macrobenthos diversity. Animal abundance macrobenthos have a very strong relationship with the content of organic matter in sediments and sedimentary textures (Kinanti et al., 2014) This means organic materials such as carbon and nitrogen affect the macrobenthos abundance.

Nitrogen cycle showing a high response to internal feedback mechanism as well as the interdependence of carbon and metal cycles. In contrast, the carbon cycle would appear mainly controlled by the decay of organic matter. Benthic carbon and nitrogen cycle has the potential to greatly affect the fertility level of water in it (Holstein and Wirtz, 2010). Macrobenthos react to changes in water quality and analysis macrobenthos is one of the most important methods to
monitor changes in water quality parameters (Cupsa et al., 2010). Putro (2007) have published about spatial and temporal patterns of the macrobenthic assemblages in relation to environmental variables.

This research will be presented as a mathematical relationship between the carbon and nitrogen to macrobenthos through a system of linear equations. For efficiency, both time and cost will be analysed Crout, LU, Cholesky decomposition and QR factorization to solve this linear equations system that requires the least mathematical operations. This can be demonstrated through a case study with data from the area of polyculture system and PT. Kayu Lapis Indonesia coastal, Mororejo village subdistrict Kaliwungu district Kendal, to choose the best method that requires the least computation time.

II. MATERIALS AND METHODS

Sampling stations were located at Mororejo village subdistrict Kaliwungu district Kendal. Location I was a cultivated area polyculture system with biota are cultivated in the polyculture ponds, i.e., fish and tiger shrimp that are cultured together with seaweed in coastal waters Mororejo village subdistrict Kaliwungu Kendal district, Central Java. Location II was the coastal area of PT. Kayu Lapis Indonesia Mororejo village subdistrict Kaliwungu district Kendal, Central Java, which is located adjacent to industrial activities as well as direct hit tide. Each location had 3 stations with 3 replicates. Sampling procedures included collecting sediments, fixation, rinsing, sorting, preservation, and identification. Sediment was analysed for sediment grain size, and total organic content.

Two-way analysis of variance was used to compare the results of measurements of physical parameters and the sediment-water chemistry between locations and times of sampling. Data were tested using Kolmogorov-Smirnov test for normal distribution of the data and Levene test for homogeneity of variance. Further post hoc test using Tukey HSD performed to further compare the results of the analysis showed a significant difference ($P<0.05$). Multivariate analysis using the principal component analysis with Euclidean distance performed to describe differences in environmental variability between sampling locations. While multivariate analysis using non-metric multi dimensional scaling using Bray-Curtis similarity was performed to the data macrobenthos to describe the differences between the location and time of sampling.

Furthermore, the data of carbon, nitrogen, and macrobenthos will bestudied mathematically through multiple linear regression model. In this case the emphasis on the process of finding the parameters of the regression equation is represented in the form of a system of linear equations. Here will be analyzed Crout, LU, Cholesky decomposition, and QR factorization methods.

III. RESULT AND DISCUSSION

3.1 Analysis of Arithmetic Operations

Comparison of the analysis of arithmetic operations is how much of the necessary arithmetic operations. In this analysis, the division will be combined with the multiplication and addition by subtraction. In this case will be compared LU, Crout, Cholesky decomposition, and QR factorization.

3.1.1 LU Decomposition Method

LU decomposition method can be explained using the following algorithm,

1. Given, matrices $A = [a_{ij}]$, $B$
2. Find $i=1, 2, ..., n$
3. Complete the matrix $L$ according to the equation $LS = B$, to find the value of $S$.
4. Complete the matrix $U$ according to the equation $LU = S$, to find the value of $Z$.

Explanation of the LU Decomposition algorithm can be seen through the flowchart in the following figure 1.

The total number of arithmetic operations for LU decomposition is,

Addition : $n^3 - 4n^2 + 9n - 7$

Multiplication : $n^3 - 7n^2 + 23n - 7$

3.1.2 Crout Decomposition Method

Crout decomposition method can be explained using the following algorithm,

1. Given, matrices $A = [a_{ij}]$, $B$
2. Find $i=1, 2, ..., n$ and $j=1,2,...,n$;
3. Complete the matrix $L$ according to the equation $LS = B$, to find the value of $S$.
4. Complete the matrix $U$ according to the equation $LU = S$, to find the value of $Z$.

Explanation of the Crout decomposition algorithm can be seen through the flowchart in the following figure 2.
The total number of arithmetic operations for Crout decomposition is:

Addition: $n^3 - 2n^2 + 2n - 1$
Multiplication : $\frac{3n^3}{2} + \frac{9n}{2} - 1$

3.1.3 QR factorization method

QR factorization method can be explained using the following algorithm,

0. Given, matrices $A = [a_{ij}]$, $B$
1. Find for $j = 1, 2, 3, ..., n$;
   
   $$q_j = \frac{w_j - \sum_{k=1}^{j-1} w_k a_{kj} a_{ij}}{\sqrt{\sum_{k=1}^{j-1} (a_{kj} a_{kj}) - (a_{kj} q_j a_{kj})}}$$
2. Find for $i = 1, 2, 3, ..., n$ and $j = 1, 2, 3, ..., n$;
   
   $$r_{ij} = q_j a_{ij}$$
3. Complete the appropriate matrix equation $Q$, from equation $QS = B$, to find the value of $S$.
4. Complete the matrix $R$ according to the equation $RZ = S$, to find the value of $Z$.

Explanation of the QR factorization algorithm can be seen through the flowchart in the following figure,

The total number of arithmetic operations for the QR factorization is,

Addition : $\frac{n^3}{2} + 2n^2 - \frac{3n}{2}$
Multiplication : $\frac{n^3}{2} + 2n^2 + n$

3.1.4 Cholesky Decomposition Method

Cholesky decomposition method can be explained using the following algorithm,

0. Given, matrices $A = [a_{ij}]$, $B$
1. Find for $i = 1$ and $j = 1$;
   
   $$l_{11} = \sqrt{a_{11}}$$
2. Find for $i=2, 3, ..., n$;
   
   $$l_{2i} = a_{2i}/l_{i1}$$
3. Find for $i=2, 3, ..., n$;
   
   $$l_{1i} = \sqrt{(a_{ii} - \sum_{p=1}^{i-1} l_{pi}^2)}$$
4. Find for $i = 2, 3, ..., n$ and $p = i+1, i+2, ..., n$;
   
   $$l_{pi} = (a_{pi} - \sum_{k=1}^{i-1} l_{kj} l_{ki})/l_{1j}$$
5. Complete the matrix $L$ according to the equation $LS = B$, to find the value of $S$.
6. Complete the appropriate matrix $L^T$ from the equation $L^T Z = S$, to find the value of $Z$.

Explanation of the Cholesky decomposition algorithm can be seen through the flowchart in the following figure,

The total number of arithmetic operations for the Cholesky decomposition is,

Addition : $\frac{n^3}{2} + 2n^2 - \frac{3n}{2}$
Multiplication : $\frac{n^3}{2} + 2n^2 + n$
4.2 SIMULATION RESULTS

The data used in this paper is the measurement data of carbon, nitrogen and macrobenthos based on research data that has been done Putro, et. al. (2014). Regression model based on the data of carbon, nitrogen and macrobenthos sequential type to forms defined variables \( X_1, X_2 \) and \( Y \). The next step, substitute the data of carbon and nitrogen into the systems of linear equations (Montgomery and Elizabeth, 1992) as follows,

\[
\begin{align*}
\sum_{i=1}^{n} X_{i1} \beta_0 + \sum_{i=1}^{n} X_{i2} \beta_1 = Y_i \\
\sum_{i=1}^{n} X_{i1} \beta_0 + \sum_{i=1}^{n} X_{i2} \beta_2 = \sum_{i=1}^{n} X_{i3} Y_i \\
\sum_{i=1}^{n} X_{i1} \beta_0 + \sum_{i=1}^{n} X_{i2} \beta_1 + \sum_{i=1}^{n} X_{i3} \beta_2 = \sum_{i=1}^{n} X_{i4} Y_i
\end{align*}
\]

Further, we find the systems of linear equations in the form,

\[
\begin{align*}
36 \beta_0 + 72.49 \beta_1 + 32.15 \beta_2 = 21.33 \\
72.49 \beta_0 + 164.17 \beta_1 + 67.28 \beta_2 = 49.88 \\
32.15 \beta_0 + 67.28 \beta_1 + 29.28 \beta_2 = 20.15
\end{align*}
\]

Rewrite the equation (3.1) in the matrix form,

\[
\begin{bmatrix}
36 & 72.49 & 32.15 \\
72.49 & 164.17 & 67.28 \\
32.15 & 67.28 & 29.28
\end{bmatrix}
\begin{bmatrix}
\beta_0 \\
\beta_1 \\
\beta_2
\end{bmatrix}
= 
\begin{bmatrix}
21.33 \\
49.88 \\
20.15
\end{bmatrix}
\]

Completion of the linear equation (3) will be calculated using the method of LU, Crout decomposition, QR factorization, and Cholesky Decomposition. Furthermore, all four methods are compared and will be analysed the most efficient method.

3.2.1 Simulation of the LU decomposition method

Finding the value of the regression model parameters can be calculated by the method of LU decomposition. Completion the systems of linear equations using LU decomposition is as follows:

1. Form the matrix A into matrices L and U matrices, suppose the above matrix with \( AZ = B \),

\[
A = \begin{bmatrix}
36 & 72.49 & 32.15 \\
72.49 & 164.17 & 67.28 \\
32.15 & 67.28 & 29.28
\end{bmatrix}, \quad Z = \begin{bmatrix}
\beta_0 \\
\beta_1 \\
\beta_2
\end{bmatrix}, \quad B = \begin{bmatrix}
21.33 \\
49.88 \\
20.15
\end{bmatrix}
\]

2. We can find the matrices L and U,

\[
U = \begin{bmatrix}
36 & 72.49 & 32.15 \\
0 & 18.2033 & 2.5424 \\
0 & 0.2136 & 0.1397
\end{bmatrix}, \quad L = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0.8931 & 0.1397
\end{bmatrix}
\]

3. The value of matrix Z from equation \( LS = B \)

\[
L = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0.8931 & 0.1397
\end{bmatrix}, \quad S = \begin{bmatrix}
21.33 \\
49.88 \\
20.15
\end{bmatrix}
\]

then, with forward substitution, we find

\[
S = \begin{bmatrix}
21.33 \\
6.9297 \\
0.1333
\end{bmatrix}
\]

4. Look for the values of parameter from equation, \( UZ = S \),

\[
\begin{bmatrix}
36 & 72.49 & 32.15 \\
0 & 18.2033 & 2.5424 \\
0 & 0 & 0.2136
\end{bmatrix}
\begin{bmatrix}
\beta_0 \\
\beta_1 \\
\beta_2
\end{bmatrix}
= 
\begin{bmatrix}
21.33 \\
6.9297 \\
0.1333
\end{bmatrix}
\]

Further, with backward substitution, we obtain

\[
Z = \begin{bmatrix}
-0.5566 \\
0.2934 \\
0.6252
\end{bmatrix}
\]

So that we have the regression model as follows,

\[
\hat{Y} = -0.5566 + 0.2934X_1 + 0.6252X_2
\]

Retrieved computing time for LU Decomposition method with MATLAB R2008a, CPU time = 1.5600 seconds.

3.2.2 Simulation of the Crout decomposition method

Finding the value of the regression model parameters can be calculated by the method of Crout decomposition. Completion the systems of linear equations using Crout decomposition is as follows:

1. Form the matrix A into matrices L and U matrix, suppose the above matrix with \( AZ = B \),

\[
A = \begin{bmatrix}
36 & 72.49 & 32.15 \\
72.49 & 164.17 & 67.28 \\
32.15 & 67.28 & 29.28
\end{bmatrix}, \quad Z = \begin{bmatrix}
\beta_0 \\
\beta_1 \\
\beta_2
\end{bmatrix}, \quad B = \begin{bmatrix}
21.33 \\
49.88 \\
20.15
\end{bmatrix}
\]

2. Then, find matrix \( L = (l_{ij}) \) and \( U = (u_{ij}) \) as follows,

\[
l_{11} = 36, \quad l_{21} = 72.49, \quad l_{31} = 32.15
\]

\[
u_{12} = a_{12}/l_{11} = 2.01361
\]

\[
u_{13} = a_{13}/l_{11} = 0.893056
\]

\[
u_{22} = a_{22} - l_{21}u_{12} = 18.20341
\]

\[
u_{23} = (a_{23} - l_{21}u_{13})/u_{22} = -0.28621
\]

\[
u_{32} = a_{32} - l_{31}u_{12} = 2.54244
\]

\[
u_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23} = 1.29592
\]

We can obtain,

\[
U = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}, \quad L = \begin{bmatrix}
36 & 0 & 0 \\
72.49 & 18.20341 & 0 \\
32.15 & 2.54244 & 1.29592
\end{bmatrix}
\]

3. Find S from equation \( LS = B \)

\[
L = \begin{bmatrix}
36 & 0 & 0 \\
72.49 & 18.20341 & 0 \\
32.15 & 2.54244 & 1.29592
\end{bmatrix}, \quad S = \begin{bmatrix}
21.33 \\
49.88 \\
20.15
\end{bmatrix}
\]

With forward substitution, can be found,

\[
S = \begin{bmatrix}
0.5925 \\
0.3807 \\
0.1028
\end{bmatrix}
\]

With backward substitution, can be found,
We have a regression model that representing the relationship carbon and nitrogen with macrobenthos diversity,
\[ \hat{Y} = -0.3251 + 0.4101X_1 + 0.1028X_2 \]

Retrieved computing time for Chelosky Decomposition method with MATLAB R2008a, CPU time = 2.2932 seconds

3.2.3 Simulation Method QR Factorization
Finding the value of the regression model parameters can be calculated by the method of QR factorization. Completion the systems of linear equations using QR factorization is as follows:
1. Form the matrix A into matrices Q and R matrices, we let the matrix above with \( AZ = B \),
\[ A = \begin{bmatrix} 36 & 72.49 & 32.15 \\ 72.49 & 164.17 & 67.28 \\ 32.15 & 67.28 & 29.28 \end{bmatrix}, Z = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, B = \begin{bmatrix} 21.33 \\ 49.88 \\ 20.15 \end{bmatrix} \]
2. We can find matrices R and Q by using MATLAB R2008a,
\[ R = \begin{bmatrix} -87,0886 & -191,453 & -80,101 \\ 0 & -8,8838 & -1,1592 \\ 0 & 0 & 0.1806 \end{bmatrix}, Q = \begin{bmatrix} -0.4134 & 0.7487 & -0.5182 \\ 0 & 0 & 0 \end{bmatrix}, \]
3. Obtain matrix S based on equation \( QS = B \),
\[ S = \begin{bmatrix} -0.5566 \\ 0.2934 \end{bmatrix} \]
4. Further, look for the values of parameter from equation \( L^T Z = S \)
\[ L = \begin{bmatrix} 6 \\ 0 \\ 0 \end{bmatrix}, S = \begin{bmatrix} 21.33 \\ 49.88 \\ 20.15 \end{bmatrix} \]

Then we find,
\[ Z = \begin{bmatrix} 3.555 \\ 1.6242 \\ 0.2887 \end{bmatrix} \]

Retrieved computing time for Chelosky Decomposition method with Matlab R2008a, CPU time = 1.4664 seconds

Furthermore, comparison of methods studied LU decomposition, Crout decomposition, QR factorization and Chelosky decomposition on arithmetic operations and computing time to solve linear equations system (4.1) that obtained from CPU time with MATLAB R2008a using a computer with processor specs: Intel (R) Atom (TM) CPU N470 @ 1.83GHz 1.83, memory: 1.99 GB, the operating system: Windows 7 in the following table,

| Method                  | Arithmetic Operations | Cputime (seconds) |
|-------------------------|-----------------------|-------------------|
| LU decomposition        | \( n^3 - 4n^2 + 9n - 7 \) | 1.5600            |
| Crout decomposition     | \( n^3 - 2n^2 + 2n - 1 \) | 2.2932            |
| QR factorization        | \( n^2 - 2n^2 + \frac{5}{2} \) | 1.5756            |
| Chelosky decomposition  | \( n^2 + \frac{n}{2} \) | 1.4664            |

We have a regression model that representing the relationship carbon and nitrogen with macrobenthos diversity, with parameter founded by QR factorization, as follows,
\[ \hat{Y} = -0.5566 + 0.2934X_1 + 0.6252X_2 \]

Retrieved computing time for Chelosky Decomposition method with MATLAB R2008a, CPU time = 1.5756 seconds

3.2.4 Simulation of the Cholesky Decomposition Method
Finding the value of the regression model parameters can be calculated by the method of Cholesky decomposition. Completion of linear equations system by using the Cholesky decomposition is as follows:
1. Form the matrix with AZ = B,
From Table 1. indicates that the most efficient method is the method of Cholesky decomposition because it has the fewest arithmetic operations. This is also verified from the calculation to determine the parameters of the regression model the relationship between carbon and nitrogen to macrobenthos diversity which calculated using MATLAB R2008a. We obtained the least of CPU time is the Cholesky decomposition of 1.4664 seconds, which means that the Cholesky decomposition is the most efficient method.

IV. CONCLUSIONS

Based on the discussion in the previous section we concluded that the result of arithmetic operations and simulation calculations using the method of LU decomposition, Crout decomposition, QR factorization and Cholesky decomposition method that the most efficient method is Cholesky decomposition. This is verified by the Cholesky decomposition method has the fewest arithmetic operations that is as much $\frac{n^3}{2} - \frac{n}{2}$ addition and $\frac{n^3}{2} + \frac{n^2}{2} + n$ multiplication.

From the simulation results to solve a system of linear equations that representing the relationship between carbon and nitrogen with the macrobenthos diversity obtained that the smallest computing time is the Cholesky decomposition i.e., 1.4664 seconds, which means that the Cholesky decomposition is the most efficient method compared by the LU, Crout decomposition, and QR factorization method.

From the regression model, we have the positive parameter this implies that abiotic factors (carbon and nitrogen) influence positively on the macrobenthos diversity, owing to the source of carbon and nitrogen as food resources of them.

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