

Jacobi Similarity Transformation for SVD and Tikhonov Regularization for Least Squares Problem: The Theoretical foundation

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Abstract: The paper presents solution to Least squares equation as driven by Singular Value Decomposition (SVD) obtained from using Jacobi Similarity Transformation without recourse to Tikhonov regularization parameter. We use the LU decomposition and QR algorithm as bases of comparison for the obtained results. A polynomial fit of order five for the Least squares problem was adopted. Sample numerical data problem was obtained as a primary source at Trodan, Kogi State University, Anyigba showing the functional relationship between Temperature and Relative Humidity. It is suggested that the SVD is numerically backward stable as attested to by the LU decomposition method relative to similar results computed by QR and other known methods.

Keywords: least squares equation, singular value decomposition, Jacobi similarity transformation algorithm, inverse problems

AMS subject Classification 65G40, 65F05

I. Introduction

In the paper we consider least squares equation as applicable to modelling many Scientific problems using SVD obtained from Jacobi Similarity Transformation, [1]. Least squares equation belongs to the class of most powerful inverse problems which deals with the process of calculating from a given set of observations the causal factors which produce them. Such situations were already often encountered in optics, radar, acoustics, communication theory and language processing, calculation of the density of the earth measurements of its gravity field, medical imaging, computer vision, oceanography, astronomy, remote sensing, machine learning and non-destructive testing, [2].

Basic tools for discussions are inverse function theorems for set valued maps, regularity points for Lipschitz function, characterization of tangential and metric regularity, and Lipschitz behaviour of multifunction in connection with a closed convex graph theorem, [3, 4].

The distance between regularity and strong regularity of set valued map $F : X \rightarrow Y$ in which the Jacobian matrix may be investigated for openness in a topological space forms the basis of our discussion. This can be verified using a theorem due to [5] which states that an interval matrix $[A]$ is strongly regular if

$\sigma_n(\text{mid}([A]_1)) > \sigma_1(\text{rad}([A]))$ which may be weak up to a factor $n^{\frac{1}{2}}$, where σ_i is the singular value of the matrix A in decreasing order. The relative distance for which a matrix A is singular to the set of singular

matrices in some norm is defined as $\text{dist}(A) = \min \left\{ \frac{\|\Delta A\|}{\|A\|} \mid (A + \Delta A) \text{ is singular} \right\}$.

The reciprocal of condition number can be interpreted as a measure of nearness to singularity of the matrix A and therefore $\text{dist}(A) = K^{-1}(A)$. As a result, [6] proved that for such a singular matrix $(A + \Delta A)$, there holds the estimate:

$$\|\Delta A\| \geq \frac{\|\Delta x\|}{\|x\|} = \frac{\|b\|}{\|A^{-1}b\|} \geq \frac{1}{\|A^{-1}\|} = \frac{\|A\|}{K(A)} \quad (1.1)$$

That is for $b = Ax$, we have

$$\frac{\|\Delta A\|}{\|A\|} \geq \frac{1}{K(A)} \quad (1.2)$$

Introduced thus into the discussion is the well known Holder's norm defined in the form

$$1 \leq \frac{\|x\|_p}{\|x\|_q} \leq n^{\frac{(q-p)}{pq}}, \left(p \leq q, \frac{1}{p} + \frac{1}{q} = 1\right) \quad (1.3)$$

Where, it is understood [7] that

$$\|x\|_q = \left\| \|x\|_p \cdot \frac{x}{\|x\|_p} \right\|_q = \|x\|_p \left\| \frac{x}{\|x\|_p} \right\|_q \leq C_{p,q} \|x\|_p \|x\|_p, \quad (1.4)$$

$C_{p,q} = \max_{\|e\|_p=1} \|e\|_q$, and $e = (e_1, e_2, \dots, e_n)^T$ is the canonical basis in R^n . This implies $\|e\|_q \leq \|x\|_p$.

By further exposition to Holder inequality would yield that:

$$\|x\|_\infty = \left(\sum_{i=1}^n |x_i|^q \right)^{\frac{1}{q}} \leq \left(n \|x\|_\infty^q \right)^{\frac{1}{q}} \leq n^{\frac{1}{q}} \|x\|_\infty \Rightarrow \lim_{q \rightarrow \infty} \|x\|_q = \|x\|_\infty ; \text{ for } \frac{1}{p} + \frac{1}{q} = 1.$$

This brings us to the concept of Lipschitz continuity for f in a manner analogous to Riemann integrable

function [8] which relates that for every norm in R^n there is $\left\| \int_a^b g(t) dt \right\| \leq \int_a^b \|g(t)\| dt$ such that :

$$\|f[x, x^{(0)}]\| = \left\| \int_0^1 f'(x^{(0)} + t(x - x^{(0)})) dt \right\| \leq \int_0^1 \|f'(x^{(0)} + t(x - x^{(0)}))\| dt \leq \int_0^1 M dt = M.$$

It follows that for a convex functional defined on $D \subset R^n$ we would expect that

$g(t) = f(x^{(0)} + t(x - x^{(0)}))$ is continuously differentiable on $[0,1]$ for which

$$\begin{aligned} f(x) - f(x^{(0)}) &= g(1) - g(0) = \int_0^1 g'(t) dt = \int_0^1 f'(x^{(0)} + t(x - x^{(0)})) (x - x^{(0)}) dt \\ &= f[x, x^{(0)}][x - x^{(0)}]. \end{aligned}$$

Wherefrom, reasons due to [9] implicated that

$\|f(x) - f(x^{(0)})\| = \|f[x, x^{(0)}]\| \|x - x^{(0)}\| \leq M \|x - x^{(0)}\|$ remain valid. More importantly, when the matrix A is a square matrix, the logarithm of A is defined by the equation

$$\log(A) = \int_0^1 (A - I)[t(A - I) + I]^{-1} dt \text{ and its condition number } K_{\log}(A) \geq \frac{K(A)}{\|\log(A)\|}.$$

The remaining part in the paper is categorized as follows: In section 2 the spectral decomposition via Jacobi similarity transformation is given a theoretical foundation. The Givens orthogonal matrix plane rotation for the construction of popular QR decomposition as a useful tool for numerical computation is highlighted. Section 3 in the paper discusses the singular value decomposition (SVD) for the least squares problem as well as Tikhonov regularization parameters in the case of singularity. In section 4 we demonstrate with numerical example with described methods. There might be need to compute zeros of polynomials; therefore section 5 in the paper presents interval Newton-Like methods for simultaneously refining all zeros of polynomial equation with particular reference to the work of [11]. Numerical illustration is demonstrated with the methods in section 6. Finally conclusion is drawn based on the strength of our findings.

II. The Spectral Decomposition via Jacobi Similarity Transformation

The importance of computing eigenvalues and eigenvectors of a real or complex matrix cannot be overemphasized in our research which is often met in physics and engineering practices, a good example is in vibration problems and analysis of variances in statistics. The Jacobi similarity transformation was derived by Jacobi in 1946 and is applicable to a real symmetric matrix A , [1, 12]. In the case the matrix is not symmetric one must first transform the matrix A to a symmetric case. The Jacobi similarity transformation matrix is based

$$a_{qq}^{(k)} = a_{pp}^{(k-1)} \sin^2 \theta - 2a_{pq}^{(k-1)} \sin \theta \cos \theta + a_{qq}^{(k-1)} \cos^2 \theta \quad (\text{By symmetry})$$

$$a_{pq}^{(k)} = (a_{pp}^{(k-1)} - a_{qq}^{(k-1)}) \cos \theta \sin \theta + (\cos^2 \theta - \sin^2 \theta) a_{pq}^{(k-1)} = a_{qp}^{(k)}$$

i.e. $a_{pq}^{(k)} = 0.0 = a_{qp}^{(k)}$ by (iv) and symmetry

$$a_{ij}^{(k)} = a_{ij}^{(k-1)} \quad \text{Elsewhere}$$

(vi) Repeat operations starting from step (ii)

Finish

Finish

End

It must be pointed out that the square root of diagonal matrix must be finally computed assuming a non symmetric matrix was originally transformed to a symmetric matrix as in the algorithm above. In a well developed sense, the Givens Rotation Orthogonal matrix [12] which is a refined Jacobi Similarity transformation obtained by Givens in 1954 for developing the QR decomposition of a symmetric matrix, where $\cos \theta$ and $\sin \theta$ respectively is computed in the form:

$$\cos \theta = \frac{p_i}{\sqrt{p_i^2 + q_i^2}}, \quad \sin \theta = \frac{q_i}{\sqrt{p_i^2 + q_i^2}}. \text{More definitive further use of Givens rotation is}$$

reduction of a symmetric matrix A to tri-diagonal form, where Sturmian sequence becomes a hand tool for the actualization of polynomial equation to which any of Newton's methods is applicable. The givens rotation is finite but Jacobi's is infinite, for exhaustive discussion on this treatise, readers are referred to [1,12]. We also pointed out that Householder Reflection can be used as an alternative putting computational cost into consideration. All the same Givens plane rotation is worthwhile in the studies of robotic arms manipulators.

III. The Least Squares Problem

The discretization of ill-posed problem often leads to linear least squares problem in the form Find $\min \|\Delta A, \Delta b\|$ such that $\min_x \|Ax - b\|_2, (A \in R^{m \times n})$ is the least squares solution of the problem.

In most experimental work which is often the case in practice, the matrix A may have a large number of singular values very close to zero. This pushes the noise which is present in b, the right hand side, to be amplified in the pseudo-inverse solution

$$x^+ = A^+ b, \quad (3.1)$$

with resultant effect of huge condition number and thereby rendering the approximate solution useless [13]. We thus introduce the Singular value decomposition (SVD) into the computation as dyadic decomposition of A :

$$A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T, \quad \text{where, } U = [U_1, U_2, \dots, U_n] \text{ is an } m \times m \text{ matrix with orthogonal column vectors,}$$

$$\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n), \quad \text{where } \sigma_n > \sigma_{n-1} > \dots > \sigma_1. \quad V \text{ is a } n \times n \text{ unitary matrix.}$$

As a result the solution process by SVD is in the form:

$$x_i = \sum_{i=1}^n \frac{c_i}{\sigma_i} v_i, \quad \text{where } c_i = u_i^T b \quad (3.2)$$

In the absence of near singularity or singularity, SVD is numerically backward stable. On the other hand if there is singularity in the solution system, there is thus, a need for development of a good number of regularization techniques [14] for which comes into focus the Tychonov regularization that replaces solution of original system

$$\min_x \left(\|Ax - b\|_2^2 + \alpha^2 \|Lx\|_2^2 \right) \quad (A \in R^{m \times n}, L \in R^{p \times n}), \quad (3.3)$$

by the nearby system

$$(A^T A + \alpha^2 I)x = A^T b \quad (3.4)$$

The parameter $\alpha \neq 0$ is a regulator which controls the weight given to the minimization of $\|Lx\|_2$ relative to the minimization of the residual $\|b - Ax\|_2$. It is supposed that $\text{rank}(L) = p \leq n \leq m$ and

$$\text{rank} \begin{pmatrix} A \\ L \end{pmatrix} = n.$$

The matrix L is a certain matrix which may be taken as an identity matrix or a discrete approximation to some derivative operator [6]. Note that in the minimization of problem 3.3, the assumption

$$\text{Null}(A) \cap \text{Null}(L) = \{O\}$$

is important for a useful purpose. In the time being, we define the **QR decomposition with matrix Q being orthogonal and R upper diagonal. The upper triangular matrixes for three different cases are outlined below:**

$$1) \quad m = n, \quad R = \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1n} \\ & r_{22} & \dots & r_{2n} \\ & & \cdot & \\ & & & \cdot \\ & & & r_{nn} \end{pmatrix},$$

$$2) \quad m < n, \quad R = \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1n} \\ & r_{22} & \dots & r_{2n} \\ & & \cdot & \\ & & & \cdot \\ & & & r_{mm} \dots r_{mn} \end{pmatrix},$$

$$3) \quad m > n, \quad R = \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1n} \\ & r_{22} & \dots & r_{2n} \\ & & \cdot & \\ & & & \cdot \\ & & & r_{mn} \\ \hline & & & & O \end{pmatrix}$$

In a note in passing, the iterated Tikhonov method with residual [6, and 17] is the equation

$$x_{k+1} = x_k + (A^T A + \alpha^2 I)^{-1} A^T (b - Ax_k), \quad k=0,1,2,\dots, \quad (3.5)$$

In the implementation of method 3.5, it is advisable as a starting point by taking $x_0 = 0$, and $x_1 = (A^T A + \alpha^2 I)^{-1} A^T b$. Indeed, mathematically, equation 3.5 has a fixed contractive gauge [15], a necessary condition for Lipschitz continuity for which the Banach Fixed point theorem is deeply implicated. We shall not delve into details here in this discussion.

IV. Numerical Experiments

Example 1.

The experimental data were taking as a primary source from TRODAN at Anyigba, Kogi State University as showed in Table 1

Table 1

S/N DATE/TIME	TEMPERATURE (θ^0) X	RELATIVE HUMIDITY (%) Y
2011-04	32.002906	67.961866
2012-04	31.331634	68.431059
2013-04	29.887573	74.096862
2010-08	27.060463	82.752606
2011-08	26.438872	83.023268
2012-08	26.191286	83.452398
2010-12	30.039266	47.560099
2011-12	28.355457	37.122311
2012-12	28.638782	50.906093
2011-02	32.267793	60.666083
2012-02	31.043251	64.010414
2013-02	31.063575	55.738473
2011-01	29.062744	32.955172
2012-01	28.816789	41.495453
2013-01	29.158118	47.972735
2010-07	26.048773	83.517390
2011-07	27.902184	79.944623
2012-07	26.945129	82.449950
2011-06	28.900817	78.000009
2012-06	27.873762	79.053775
2011-03	33.950121	60.316848
2012-03	33.401677	54.788059
2013-03	33.303313	65.349271
2011-05	30.639803	73.495656
2012-05	29.369926	75.301975
2010-11	29.471345	76.122503
2011-11	28.170606	66.909216
2012-11	28.891984	76.298347
2010-10	28.214158	80.737601
2011-10	27.204551	80.169298
2012-10	27.401785	81.294369
2010-09	27.053905	82.342825
2011-09	26.616421	81.995541
2012-09	26.590674	83.569152

It is suggested that Temperature in θ^0 is independent variable X and that Relative Humidity is the dependent variable Y. We use windows 2007 version of MATLAB for the calculations and set of results in floating point arithmetic is displayed in Table 2.

Table 2 showing Results computed for the considered methods

LU decomposition method for (3.1) \hat{x}	QR decomposition method for (3.1) \hat{x}	Singular decomposition (3.2) \hat{x}	value method	Tikhonov Regularization method 3.4 with $\alpha \in [0.01, 0.1]$. \hat{x}
1.0e+006*	1.0e+009*	1.0e+006*		1.0e - 003 *
$\begin{pmatrix} -1.4607 \\ 0.2449 \\ -0.0164 \\ 0.0005 \\ -0.0000 \\ 0.0000 \end{pmatrix}$	$\begin{pmatrix} 0.0000 \\ 0.0001 \\ 0.0034 \\ -0.1122 \\ -1.6977 \\ 9.7780 \end{pmatrix}$	$\begin{pmatrix} -1.4209 \\ 0.2380 \\ -0.0159 \\ 0.0005 \\ -0.0000 \\ 0.0000 \end{pmatrix}$		$\begin{pmatrix} 0.0000 \\ 0.0000 \\ -0.1620 \\ 0.1320 \\ 0.0160 \\ 0.0020 \end{pmatrix}$

In Table 2 computed results for LU decomposition and Singular Value decomposition (SVD) are numerically backward stable with high degree of closeness when compared with results from QR Factorization. On the other hand, the Tikhonov regularization method seemed to have performed very poorly in this case which was quite unexpected. We took the parameter λ in the interval of $[0.01, 0.1]$ and found out that there was no significant difference in the results as all computed results by Tikhonov regulated parameter method in the interval stated were the same. The graph illustrating the above results can be demonstrated using MATLAB plot function as displayed in Figures 1-3. Each of the methods in the figures was referred to Series 1,2,3 and 4 respectively. That is to say, the LU method (Series 1), QR method (series 2), SVD method (series 3), and Tikhonov regularization method (series 4). Computationally the ill-posed problem implicated that $0 \in \sigma(A^T A)$, the spectrum of $A^T A$ an indication that eigenvalues of $(A^T A)^{-1}$ are unbounded. This means that for some i , there is $n(\lambda_i) < m(\lambda_i)$, hence the matrix $A^T A$ is degenerated, thus, the eigenvectors and principal vectors derive the Jordan form of $A^T A$, [12].

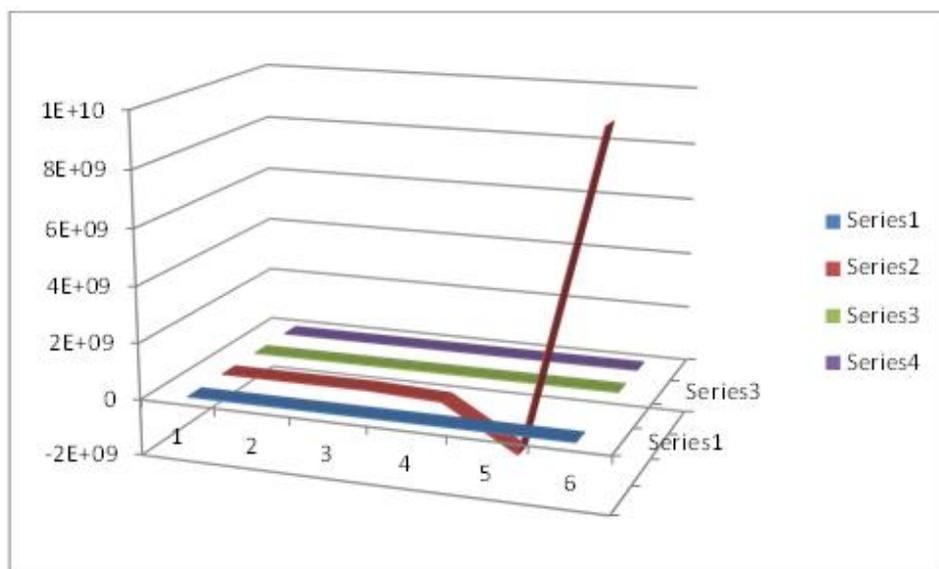


Figure 1

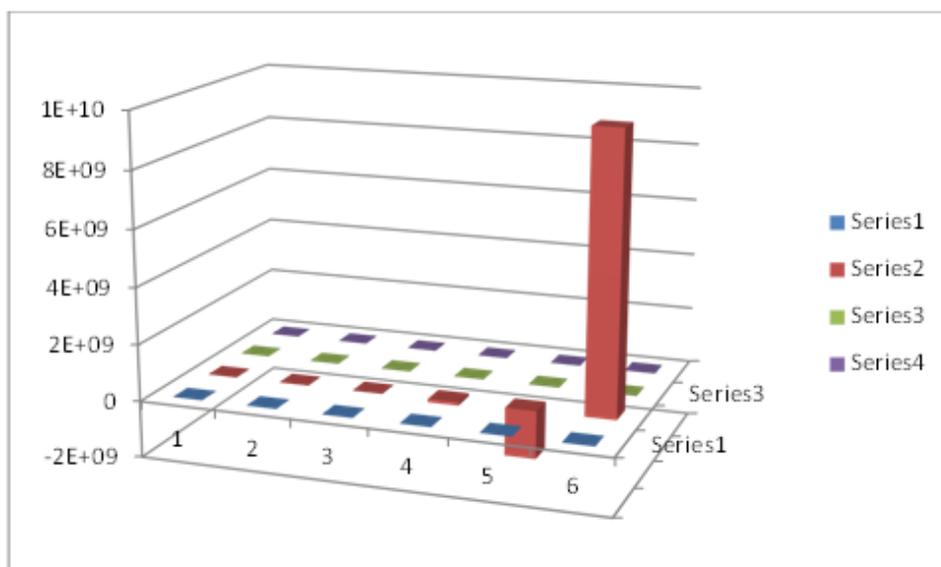


Figure 2

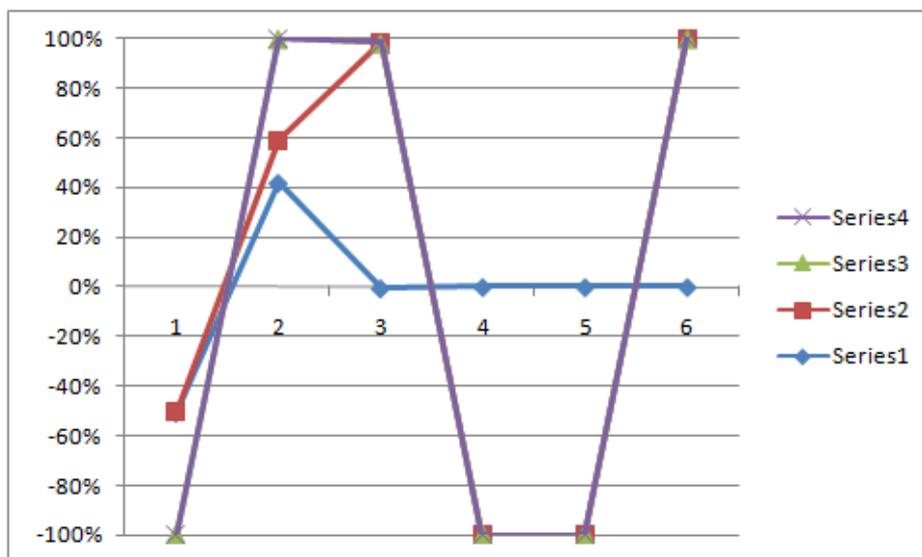


Figure. 3

V. Computation of polynomial zeros by the Interval Newton Operator

Supposing the coefficients appearing in the polynomial fit for the least squares problems are expressed in the form of uncertainty such that:

$$P(t) = \sum_{j=0}^n a^j t^j = a_0 + a_1 t + \dots + a_{n-1} t^{n-1} + a_n t^n \quad (\text{where } a_j \text{ are real or complex.}) \quad (5.1)$$

If we normalize the above polynomial equation, a monic polynomial with leading coefficient unity is obtained. The Newton operator for single variable equation as applicable to the work is given in the form

$$t_i^{(k+1)} = t_i^{(k)} - \left(p'(t_i^{(k)}) \right)^{-1} p(t_i^{(k)}), \quad k = 0, 1, 2, \dots, \quad (5.2)$$

Let T_0 be a non empty convex subset of a Banach space and let p be a contraction of T_0 into itself. If there is a compact set $N \subset T_0$ such that $N = \{p(t) : t \in N\}$ and N has at least two points, then there exists a non empty closed convex set K such that:

$$p(t) \in K_i \cap T_0 \quad \forall t \in K_i \cap T_0 \quad \text{and} \quad N \cap K_i \neq \emptyset \quad (K_i \text{ is the complement of } K_i).$$

It is supposed that pair of points is separated, that is, they are in T_2 - space and Lindelof condition for computability axiom holds. By Tietze extension theorem, it would follow that T is normal and $t \subset T$ is closed, thus every continuous function $p : t \rightarrow R$ extends to a continuous function on T . If we relate closely with Hahn-Banach extension theorem, then we would link regularity spaces with normality via Urysohn's metrization theorem that is afforded by Tychonoff so that the closed graph theorem and uniform boundedness principle, the pillars of Baire's category are in force for which the basic principle for finding zeros of polynomial holds. It is expected the unit ball $B^* \subset D$ is also compact in the weak star topology. The theoretical foundation as earlier mentioned at the beginning dedicated to the work [11] is as follows. For a monic polynomial of degree n whose zeros $\zeta_1, \zeta_2, \dots, \zeta_r$ ($r \leq n$) of respective multiplicities $\mu_1, \mu_2, \dots, \mu_r$ are known, we define that

$$P(t) = \prod_{j=1}^r (t - \zeta_j)^{\mu_j} \quad (5.2)$$

Introduce the following notations in the sense of [16,17] that:

$$\Sigma_{v,i} = \sum_{\substack{j=1 \\ j \neq i}}^r \frac{\mu_j}{(t_i - \zeta_j)^v} \quad (v = 1, 2);$$

$$\varphi_i = n\Sigma_{2,i} - \frac{n}{n - \mu_i} \Sigma_{1,i}^2;$$

$$\delta_{1,i} = \frac{p'(t_i)}{p(t_i)}, \quad \delta_{2,i} = \frac{p'(t_i)^2 - p(t_i)p''(t_i)}{p(t_i)^2};$$

$$\varepsilon_i = t - \zeta_i.$$

By further using ideas due to [9,16,and 17] it would be obtained that

$$n\delta_{2,i} - \delta_{1,i}^2 - \varphi_i = \frac{\mu_i}{n - \mu_i} \left(\frac{n}{\varepsilon_i} - \delta_{1,i} \right)^2 \quad (5.3)$$

The fixed point relation of Laguerrel’s type method can be developed [16] wherefrom:

$$\zeta_i = t_i - \frac{n}{\delta_{1,i} \pm \left[\left(\frac{n - \mu_i}{\mu_i} \right) \left(n\delta_{2,i} - \delta_{1,i}^2 - \varphi_i \right) \right]^{\frac{1}{2}}}$$

$$= t_i - \frac{n}{\delta_{1,i} \pm \left[\left(\frac{n - \mu_i}{\mu_i} \right) \left(n\delta_{2,i} - \delta_{1,i}^2 - n\Sigma_{2,i} + \frac{n}{(n - \mu_i)} \Sigma_{1,i}^2 \right) \right]^{\frac{1}{2}}} \quad (5.4)$$

In the case of simple zeros, $\mu_1 = \mu_2 = \dots = \mu_n = 1$, formula expressed in equation 5.4 is the familiar Laguerrel’s method of third order of convergence. The choice of the two roots to be taken from the two disks in equation 5.4 is guided by the discussion detailed in [16]. Implementation of the above in Circular interval arithmetic by simultaneously refining the zeros of the polynomial equation $P(t) = 0$ where the midpoint and radius of the refining disk should intersect, and taking into consideration that t_i is a new approximation to the zeros $\zeta_1, \zeta_2, \dots, \zeta_r$ of P is written in the form:

$$t_i^{(k+1)} = t_i^{(k)} - \frac{n}{\delta_{1,i}^{(k)} + \left[\left(\frac{n - \mu_i}{\mu_i} \right) \left(n\delta_{2,i}^{(k)} - (\delta_{1,i}^{(k)})^2 - f_i^{(k)} \right) \right]^{\frac{1}{2}}} \quad (5.5)$$

$$(i \in I_r), k = 0, 1, \dots, t_i^{(k)} \in \text{mid}T_i^{(k)}.$$

In Equation 5.4, $f_i^{(k)} = nS_{2,i} - \frac{n}{n - \mu_i} S_{1,i}^2$, $S_{1,i}^2 = \sum_{\substack{j=1 \\ j \neq i}}^r \frac{\mu_j}{(t_i - t_j)^2}$, $S_{2,i} = \sum_{\substack{j=1 \\ j \neq i}}^r \frac{\mu_j}{(t_i - t_j)^2}$.

We noted that a version of the iterative method of Halley type in the case of simple zeros in equation 5.2 is given by the equation:

$$t^{(k+1)} = t^{(k)} - \frac{p(t^{(k)})}{p'(t^{(k)})} \left[1 + \frac{p(t^{(k)})p''(t^{(k)})}{2p'(t^{(k)})^2} \right], k=0,1,\dots, \quad (5.6)$$

The number of multiplicities of the roots in a given disk $ID_0 \subset R$ in the sense of [17], is the Lagouanell limiting formula as derived in [18] in the form:

$$t \xrightarrow{\lim} \zeta \frac{d}{dt} \left(\frac{1}{D(t)} \right) = t \xrightarrow{\lim} \zeta \frac{d}{dt} \left(\frac{p'(t)}{p(t)} \right) = t \xrightarrow{\lim} \zeta \left| \frac{p''(t)p(t) - p'(t)^2}{p(t)^2} \right| \quad (5.6)$$

Where $|t|$ denotes the integer closest to the real number t.

VI. Conclusion

The paper studied use of singular value decomposition obtained from Jacobi similarity transformation for the solution of least squares problem. We compared notes with similar results computed by the LU Factorization and QR algorithm. Sample numerical example was taken as primary source data from TRODAN, Centre for Lower Atmospheric Studies, Kogi State University, Anyigba, Kogi State, Nigeria for the Temperature and Relative Humidity for a period of Thirty four months which was the time range the Centre for Lower atmospheric Studies was established. A polynomial fit of order five was used. Numerical results computed by the above named methods are given in Table 2. We also illustrated the results computed for the purpose of forecasting as shown in Figures 1-3. It is suggested that there is a strong correlation in the data as seen from Figure 3 as a result of colinearity between LU decomposition and SVD. An efficient interval based method for simultaneously refining zeros of polynomial when coefficients are expressed in the form of uncertainty was discussed in the sense Petkovic [11, 16] for the purpose of easy accessibility to the readers.

In computing with Jacobi method, one first transforms a non symmetric matrix to a symmetric matrix. It is recommended that when a matrix A is nearly diagonal, Jacobi similarity transformation method will always have an upper hand over QR method provided that proper stopping criterion is specified for Jacobi's method [6].

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