Lanczos algorithm of minimized iterations

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Abstract

We give an elementary exposition of the Lanczos technique to solve the matrix eigenvalue problem. This Lanczos procedure is one of the most frequently used numerical methods in matrix computations, and it is one of the 10 algorithms that exerted the greatest influence in the development and practice of science and engineering in the 20th century.

Keywords: Lanczos method, Algebraic eigenvalue problem, Conjugate gradient method.

Resumen

Damos una exposición elemental de la técnica de Lanczos para resolver el problema de valores propios de una matriz. Este procedimiento de Lanczos es uno de los métodos numéricos más empleados en cálculos matriciales, y fue seleccionado como uno de los 10 algoritmos que ejercieron la mayor influencia en el desarrollo y práctica de la ciencia e ingeniería en el Siglo XX.

Palabras clave: Método algebraico de Lanczos, problema de valores propios, método del gradiente conjugado.

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I. INTRODUCTION

At the time of Lanczos work on the eigenvalue problem during the Second World war, most methods focused on finding the characteristic polynomial [1, 2] of matrices in order to find their eigenvalues. In fact, Lanczos original paper [3] was also mostly concerned with this problem, however, he was trying to reduce the round-off errors in such calculations. He called his procedure the 'method of minimized iterations' [4]. With the first implementations of the Lanczos algorithm on the computers of the 1950's, an undesirable numerical phenomenon was encountered. Due to the finite precision arithmetic, after some number of steps the orthogonality among the Lanczos vectors was lost. This situation may be avoided by additional labor to maintain the orthogonality. In exact arithmetic, the Lanczos technique can find only one eigenvector of a multiple eigenvalue. The block methodology introduced by Golub-Underwood [5] working with multiple Lanczos vectors at a time, results in accurate calculation of multiple eigenvalues.

Calculating the inverse of a matrix [6, 7] proved to be a somewhat difficult task. To avoid matrix inversion, determined the matrix characteristic polynomial [8, 9, 10, 11, 12] was a preferred method. The roots of this polynomial provided the eigenvalues. Lanczos [3, 4] developed a progressive algorithm for the gradual construction of the characteristic polynomial. Starting from a trial vector and applying matrix transformations, Lanczos generated an iterated sequence of linearly independent vectors, each of them being a linear combination of the previous vectors. The procedure automatically comes to a halt when the proper degree of the polynomial has been reached. The coefficients of the final linear combination of the iterated vectors provide the coefficients of the characteristic polynomial.

While Lanczos was working on his paper [3], A. M. Ostrowski [13] pointed out to Lanczos that his eigenvalue method paralleled the earlier research of Krylov [14]. Lanczos checked the relevant reviews in the reference journal Zentralblatt and informed Ostrowski that the literature available to him showed no evidence that the eigenvalue algorithm and the results he obtained have been found earlier. Using matrix transformation, Krylov created a sequence of consecutive vectors that had the smallest set of consecutive iterates that are linearly dependent. The coefficients of a vanishing combination are the coefficients of a divisor of the characteristic polynomial of the matrix. The space these vectors determine is called the Krylov subspace. Krylov's iterative solver generated a huge class of approximate methods, among which the Lanczos algorithm [15] today is one of the most frequently used numerical methods in matrix computations [16].

Lanczos received credit for its discovery [17] because in 2000, the Editors of 'Computing in Science and Engineering', composed a list of 10 algorithms that exerted the greatest influence on the development and practice of science and engineering in the 20th century [18]; the Lanczos method was selected. Lanczos [3, 4] and Hestenes-Stiefel [19] initiate the implementation of Krylov subspace iteration techniques [6].

II. LANCZOS METHOD: MINIMUM POLYNOMIAL, EIGENVALUES AND EIGENVECTORS

The Lanczos algorithm generates a set of orthogonal vectors which satisfy a recurrence relation. It connects three consecutive vectors with the result that each newly generated vector is orthogonal to all of the previous ones. The numerical constants of the relation are determined during the process from the condition that the length of each newly produced vector should be minimal. After a minimum number of iterations (minimized iterations) in view of the Cayley-Hamilton-Frobenius identity [1, 2, 20], the last vector must become a linear combination of the previous vectors. The method, though indisputably an elegant one, had a serious limitation. In case of eigenvalues with considerable dispersion, the successive iterations will increase the gap, the large proper values will monopolize the scene, and because of rounding errors the small eigenvalues begin to lose value. After a few iterations they will be practically drowned out. A certain kind of eigenvalue identity had to be established. Lanczos developed a modification of the method that protected the small proper values by balancing the distribution of amplitudes in the most equitable fashion. To achieve this, the coefficients of the linear combination of the iterated vectors are determined in such a way that the amplitude of the new vector should be minimal. The generated vectors were orthogonal to each other (successive orthogonalization).

Lanczos first considered symmetric matrices, $A = A^T$, and set out to find the characteristic polynomial $P(\lambda) = \det(\lambda I - A)$ for the eigenvalue problem $A\vec{u} = \lambda\vec{u}$, and he generates a sequence of trial vectors, resulting in a successive set of polynomials. The process starts with $\vec{b}_0$ randomly selected, it may be unitary ($\vec{b}_0^T\vec{b}_0 \equiv \vec{b}_0\cdot\vec{b}_0 = 1$) to simplify some expressions, then we construct the next vector in according with the rule

$$\vec{b}_1 = A\vec{b}_0 - \alpha_0\vec{b}_0\,, \qquad (1)$$

where the value of α_0 must imply that $\vec{b}_1^2$ is a minimum, thus

$$\alpha_0 = \vec{b}_0\cdot A\vec{b}_0\,, \quad \vec{b}_0\cdot\vec{b}_1 = 0\,, \quad \vec{b}_0^2 = 1\,, \qquad (2)$$

being $\vec{b}_1$ orthogonal to $\vec{b}_0$. Similarly,

$$\vec{b}_2 = A\vec{b}_1 - \alpha_1\vec{b}_1 - \beta_0\vec{b}_0\,, \qquad (3)$$

with the parameters α_1 and $\vec{\beta}_0$ such that $\vec{b}_2^2$ has a minimum value, therefore:

$$\vec{b}_1^2\,\alpha_1 = \vec{b}_1\cdot A\vec{b}_1\,, \quad \beta_0 = \vec{b}_0\cdot A\vec{b}_1\,, \quad \vec{b}_2\cdot\vec{b}_0 = \vec{b}_2\cdot\vec{b}_1 = 0, \qquad (4)$$

and

$$\vec{b}_3 = A\vec{b}_2 - \alpha_2\vec{b}_2 - \beta_1\vec{b}_1\,, \qquad \vec{b}_2^2\,\alpha_2 = \vec{b}_2\cdot A\vec{b}_2\,,$$

$$\vec{b}_1^2\,\beta_1 = \vec{b}_1\cdot A\vec{b}_1\,, \qquad (5)$$

for a minimum value of $\vec{b}_3^2$ with $\vec{b}_3\cdot\vec{b}_r = 0$, r = 0, 1, 2, etc. The algorithm established by Lanczos is now:

$$\begin{array}{lll} \vec{b}_0 \text{ randomly selected vector,} & \vec{b}_0^2 = 1, & A = A^T, \\ \vec{b}_1 = (A - \alpha_0 I)\,\vec{b}_0\,, & \vec{b}_2 = (A - \alpha_1 I)\,\vec{b}_1 - \beta_0\,\vec{b}_0\,, & \vec{b}_3 = (A - \alpha_2 I)\,\vec{b}_2 - \beta_1\,\vec{b}_1\,, \\ \vdots & \vdots & \vdots \\ \vec{b}_m = (A - \alpha_{m-1} I)\,\vec{b}_{m-1} - \beta_{m-2}\,\vec{b}_{m-2} = \vec{0} & & \text{(end of the process)}, \end{array} \qquad (6)$$

this is the famous three-member recurrence [15], where:

$$\vec{b}_r^2\,\alpha_r = \vec{b}_r\cdot A\vec{b}_r\,,\ r = 0, 1, \ldots, m\text{-}1,$$

$$\vec{b}_q^2\,\beta_q = \vec{b}_q\cdot A\vec{b}_{q+1}\,,\ q = 0, 1, \ldots, m\text{-}2,$$

$$\vec{b}_a\cdot\vec{b}_c = 0\,, \quad a = 1, 2, \ldots, m\text{-}1;\ c = 0, 1, \ldots, a\text{-}1. \qquad (7)$$

In general, at every step of the Lanczos method a new $\vec{b}_{j+1}$ vector is found by projecting the $A\vec{b}_j$ vector into the subspace spanned by the previous Lanczos vectors and choosing $\vec{b}_{j+1}$ to be the component of $A\vec{b}_j$ orthogonal to the projection. In Lanczos view we reached the order of the minimal polynomial [21, 22, 23]:

$$m \le n \quad \text{for} \quad A_{nxn} = A^T.$$

Unfortunately, in finite precision arithmetic, the process may reach a state where β_k is very small for $k < m$ before the full order of the minimum polynomial is obtained. This phenomenon, at the time not fully understood, contributed to the method's bad numerical reputation in the 1960's.

This algorithm generates a sequence of polynomials to construct the minimum polynomial of a symmetric matrix:

$$p_0(\lambda) = 1\,, \quad p_1(\lambda) = \lambda - \alpha_0\,, \quad p_2(\lambda) = (\lambda - \alpha_1)\, p_1(\lambda) - \beta_0\, p_0(\lambda)\,, \quad \ldots \quad p_r(\lambda) = (\lambda - \alpha_{r-1})\, p_{r-1}(\lambda) - \beta_{r-2}\, p_{r-2}(\lambda)\,, \quad r = 2, 3, \ldots, \tag{8}$$

then the minimal polynomial of A is given by:

$$p_m(\lambda) = (\lambda - \alpha_{m-1})\, p_{m-1}(\lambda) - \beta_{m-2}\, p_{m-2}(\lambda)\,, \tag{9}$$

where m was determined in the process (6) ($\vec{b}_m = \vec{0}$). For example, if

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \tag{10}$$

we may select

$$\vec{b}_0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \;\therefore\; \vec{b}_0^2 = 1\,,\; A\vec{b}_0 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},\; \alpha_0 = 1\,,$$

and from (6, 7):

$$\vec{b}_1 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},\; \vec{b}_1^2 = 1\,,\; \vec{b}_1 \cdot \vec{b}_0 = 0\,,\; A\vec{b}_1 = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix},$$

$$\alpha_1 = -1\,,\; \beta_0 = 1\,,\; \vec{b}_2 = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix},\; \vec{b}_2^2 = 1\,,$$

$$\vec{b}_2 \cdot \vec{b}_0 = \vec{b}_2 \cdot \vec{b}_1 = 0\,,\; A\vec{b}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},\; \alpha_2 = 0\,,$$

$$\beta_1 = 1\,,\; \vec{b}_3 = \vec{0},$$

then m = 3 and (8, 9) imply the polynomials $p_0 = 1, p_1 = \lambda - 1, p_2 = \lambda^2 - 2$, therefore (10) has the minimal polynomial:

$$p_3(\lambda) = \lambda\,(\lambda^2 - 2) - (\lambda - 1) = \lambda^3 - 3\lambda + 1, \tag{11}$$

in this case it coincides with the characteristic polynomial. For the symmetric matrix:

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{12}$$

we select $\vec{b}_0^T = (1\ 0\ 0)$, then

$$\alpha_0 = \alpha_1 = 0, \quad \beta_0 = 1, \quad \vec{b}_1 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \vec{b}_1 \cdot \vec{b}_0 = 0,$$

$$\vec{b}_2 = \vec{0}, \quad m = 2,$$

therefore $p_0 = 1$, $p_1 = \lambda$, with the minimal polynomial $p_2(\lambda) = \lambda^2 - 1$, in harmony with the identity $A^2 = I$ verified by (12). In this example the characteristic polynomial is given by:

$$P(\lambda) = (\lambda - 1)\, p_2(\lambda) = (\lambda - 1)^2(\lambda + 1) = \lambda^3 - \lambda^2 - \lambda + 1. \tag{13}$$

Remark 1: The trial vector $\vec{b}_0$ is unitary, then it is easy to prove that $\vec{b}_1^2 = \beta_0, \vec{b}_2^2 = \beta_0\beta_1, \vec{b}_3^2 = \beta_0\beta_1\beta_2$,…, thus, in general $\vec{b}_r^2 \neq 1$, r = 1, 2,…

Remark 2: From (8), the Lanczos polynomials may be expressed as determinants of matrices generated by the parameters (7), in fact

$$p_r(\lambda) = \det\,(\lambda\, I_{rxr} - L_{rxr})\,,\; r = 1, 2, 3, \ldots \tag{14}$$

with the tridiagonal matrix [24]:

$$L = \begin{pmatrix} \alpha_0 & \beta_0 & 0 & \cdots & 0 \\ 1 & \alpha_1 & \beta_1 & \cdots & \\ 0 & 1 & \alpha_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ 0 & 0 & 0 & 1 & \alpha_{r-1} \end{pmatrix}, \tag{15}$$

that is

$$L_{1x1} = (\alpha_0)\,, \quad L_{2x2} = \begin{pmatrix} \alpha_0 & \beta_0 \\ 1 & \alpha_1 \end{pmatrix},$$

$$L_{3x3} = \begin{pmatrix} \alpha_0 & \beta_0 & 0 \\ 1 & \alpha_1 & \beta_1 \\ 0 & 1 & \alpha_2 \end{pmatrix},\; L_{4x4} = \begin{pmatrix} \alpha_0 & \beta_0 & 0 & 0 \\ 1 & \alpha_1 & \beta_1 & 0 \\ 0 & 1 & \alpha_2 & \beta_2 \\ 0 & 0 & 1 & \alpha_3 \end{pmatrix}.$$

For nonsymmetric matrices, the transpose of A participates in the implementation of the Lanczos technique, thus $\vec{b}_0$ and $\vec{t}_0$ are randomly selected vectors with $\vec{b}_0 \cdot \vec{t}_0 = 1$ to construct:

$$\vec{b}_1 = A\vec{b}_0 - \alpha_0\vec{b}_0\,, \qquad \vec{t}_1 = A^T\vec{t}_0 - \alpha_0\vec{t}_0\,,$$

$$\vec{b}_1 \cdot \vec{t}_0 = \vec{t}_1 \cdot \vec{b}_0 = 0\ , \tag{16}$$

Then

$$\alpha_0 = \vec{b}_0 \cdot A^T \vec{t}_0 = \vec{t}_0 \cdot A \vec{b}_0\ . \tag{17}$$

Similarly,

$$\vec{b}_2 = A\vec{b}_1 - \alpha_1 \vec{b}_1 - \beta_0 \vec{b}_0,\ \vec{t}_2 = A^T \vec{t}_1 - \alpha_1 \vec{t}_1 - \beta_0 \vec{t}_0, \tag{18}$$

such that $\vec{b}_2 \cdot \vec{t}_q = \vec{t}_2 \cdot \vec{b}_q = 0$, q = 1, 2, therefore:

$$\vec{b}_1 \cdot \vec{t}_1\ \alpha_1 = \vec{b}_1 \cdot A^T \vec{t}_1 = \vec{t}_1 \cdot A \vec{b}_1\ ,$$

$$\beta_0 = \vec{b}_1 \cdot A^T \vec{t}_0 = \vec{t}_1 \cdot A \vec{b}_0\ , \tag{19}$$

in general, for r = 0, 1, 2,… :

$$\vec{b}_{r+2} = A\vec{b}_{r+1} - \alpha_{r+1} \vec{b}_{r+1} - \beta_r \vec{b}_r\ ,$$

$$\vec{t}_{r+2} = A^T \vec{t}_{r+1} - \alpha_{r+1} \vec{t}_{r+1} - \beta_r \vec{t}_r\ ,$$

$$\vec{b}_r \cdot \vec{t}_r\ \alpha_r = \vec{b}_r \cdot A^T \vec{t}_r = \vec{t}_r \cdot A \vec{b}_r\ , \tag{20}$$

$$\vec{b}_r \cdot \vec{t}_r\ \beta_r = \vec{b}_{r+1} \cdot A^T \vec{t}_r = \vec{t}_{r+1} \cdot A \vec{b}_r\ ,$$

$\vec{b}_a \cdot \vec{t}_c = \vec{t}_a \cdot \vec{b}_c = 0$, a = 1, 2,…, m-1 ;

c = 0, 1,…, a-1 (biorthogonality),

this process stops when $\vec{b}_m = \vec{t}_m = \vec{0}$, $m \le n$, and the minimal polynomial of A is given by (8, 9) with the parameters α_r and β_r determined in (20). If $A = A^T$, then the expressions (16,…, 20) imply (1,…, 7) because $\vec{b}_r = \vec{t}_r$.

For example, if

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 2 & 0 \end{pmatrix}, \tag{21}$$

we may select the trial vectors:

$$\vec{b}_0 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \vec{t}_0 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \ \therefore\ \vec{b}_1 = \begin{pmatrix} -2 \\ -2 \\ 2 \end{pmatrix},\ \vec{t}_1 = \begin{pmatrix} -2 \\ 2 \\ -3 \end{pmatrix},$$

$$\alpha_0 = 3,\ \alpha_1 = -2,\ \beta_0 = -6,\ \ \vec{b}_2 = \vec{t}_2 = \vec{0},\ \ m = 2,$$

and from (8, 9)

$$p_0 = 1, \qquad p_1 = \lambda - 3,$$

$$p_2(\lambda) = \lambda^2 - \lambda\text{: Minimal polynomial,} \tag{22}$$

compatible with the relation $A^2 = A$ satisfied by (21).

Now let

$$A = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{23}$$

with the initial vectors:

$$\vec{b}_0 = \begin{pmatrix} -1 \\ 1 \\ 4 \end{pmatrix},\ \vec{t}_0 = \begin{pmatrix} 0 \\ -1 \\ \frac{1}{2} \end{pmatrix}\ \therefore\ \vec{b}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},\ \vec{t}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},$$

$$\alpha_0 = \alpha_2 = \beta_0 = 1,\ \ \alpha_1 = 0,\ \ \beta_1 = -2, \tag{24}$$

$$\vec{b}_2 = \begin{pmatrix} 2 \\ -2 \\ -4 \end{pmatrix},\ \vec{t}_2 = \begin{pmatrix} 0 \\ 2 \\ -1/2 \end{pmatrix},\ \vec{b}_3 = \vec{t}_3 = \vec{0},\ m = 3,$$

and the sequence of polynomials

$$p_0 = 1, \quad p_1 = \lambda - 1, \quad p_2 = \lambda^2 - \lambda - 1,$$

$$p_3(\lambda) = \lambda^3 - 2\lambda^2 + 2\lambda - 1\text{: Characteristic polynomial.} \tag{25}$$

Remark 3: Due to the finite precision arithmetic, after some number of steps the biorthogonality of the Lanczos vectors is lost, it is necessary additional work to maintain the orthogonality during the process.

Remark 4: The characteristic polynomial permits to obtain the eigenvalues λ_j of a matrix. The quantities $p_c(\lambda_j)$ and $\vec{b}_r \cdot \vec{t}_r$ are important to determine the corresponding eigenvectors.

Lanczos used the characteristic polynomial developed above and the biorthogonality of the $\vec{b}_r, \vec{t}_r$ sequence to find an explicit solution for the eigenvectors in terms of these trial vectors. We consider an arbitrary matrix A_{nxn} with rank A = n; its eigenvalue problem is complete if its transpose participates in the process:

$$A\vec{u}_r = \lambda_r \vec{u}_r\ , \quad A^T \vec{v}_r = \lambda_r \vec{v}_r\ , \quad r = 1, 2, \ldots, n \tag{26}$$

because both matrices have the same characteristic polynomial [1]. If we accept that:

$$Q_j \equiv \vec{b}_j \cdot \vec{t}_j \ne 0\ , \quad j = 0, 1, \ldots, n\text{-}1, \tag{27}$$

then the Lanczos algorithm gives expressions to construct their n linearly independent eigenvectors:

$$\vec{u}_k = \frac{1}{Q_0} \vec{b}_0 + \frac{p_1(\lambda_k)}{Q_1} \vec{b}_1 + \frac{p_2(\lambda_k)}{Q_2} \vec{b}_2 + \ldots + \frac{p_{n-1}(\lambda_k)}{Q_{n-1}} \vec{b}_{n-1}\ ,$$

$$k = 1, \ldots, n, \tag{28}$$

$$\vec{v}_k = \frac{1}{Q_0} \vec{t}_0 + \frac{p_1(\lambda_k)}{Q_1} \vec{t}_1 + \frac{p_2(\lambda_k)}{Q_2} \vec{t}_2 + \ldots + \frac{p_{n-1}(\lambda_k)}{Q_{n-1}} \vec{t}_{n-1}\ ,$$

with the known property [1] $\vec{u}_j \cdot \vec{v}_k = 0, j \neq k$, that is:

$$\sum_{r=0}^{n-1} \frac{1}{Q_r}\, p_r(\lambda_q)\, p_c(\lambda_c) = 0, \;\; q \neq c. \tag{29}$$

For example, the matrix (23) has the characteristic polynomial (25) whose roots are:

$$\lambda_1 = 1, \quad \lambda_2 = \left(\frac{1}{2}\right)\left(1 - i\sqrt{3}\right),$$

$$\lambda_3 = \left(\frac{1}{2}\right)\left(1 + i\sqrt{3}\right). \tag{30}$$

Therefore

$$p_1(\lambda_1) = 0, \quad p_1(\lambda_2) = -\lambda_3, \quad p_1(\lambda_3) = -\lambda_2,$$

$$p_2(\lambda_1) = -1, \quad p_2(\lambda_2) = -2, \quad p_2(\lambda_3) = -2, \tag{31}$$

$$Q_0 = 1, \qquad Q_1 = 1, \qquad Q_2 = -2,$$

in according with (29), and from (24, 28, 31) the eigenvectors are:

$$\vec{u}_1 = \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}, \quad \vec{u}_2 = \begin{pmatrix} \lambda_2 \\ -1 \\ 0 \end{pmatrix}, \quad \vec{u}_3 = \begin{pmatrix} \lambda_3 \\ -1 \\ 0 \end{pmatrix},$$

$$\vec{v}_1 = \begin{pmatrix} 0 \\ 0 \\ 1/4 \end{pmatrix}, \quad \vec{v}_2 = \begin{pmatrix} -\lambda_3 \\ \lambda_2 \\ 0 \end{pmatrix}, \quad \vec{v}_3 = \begin{pmatrix} -\lambda_2 \\ \lambda_3 \\ 0 \end{pmatrix}. \tag{32}$$

Remark 5: This Lanczos-Hestenes-Stiefel method was originally developed as a direct algorithm to solve an *n* x *n* linear system, and it is useful when employed [25] as an iterative approximation technique for solving large sparse systems with nonzero entries occurring in predictable patterns. These problems frequently arise in the solution of boundary-value problems; good results are obtained in only about $\sqrt{n}$ iterations. Employed in this way, the method is preferred over Gaussian elimination.

Remark 6: The Lanczos procedure solves the standard eigenvalue problem (26) for square matrices, then it must be interesting to realize its implementation for the rectangular case known as 'shifted eigenvalue problem' [26, 27, 28, 29].

Remark 7: The iterative Faddeev's method [6, 30, 31] permits to determine the inverse matrix A^{-1}, however, Lanczos algorithm gives us an alternative way for the inversion of a matrix. In fact, we construct the *n* x *n* matrices:

$$B = \left(\frac{\vec{b}_0}{Q_0}\, \frac{\vec{b}_1}{Q_1} \ldots \frac{\vec{b}_{n-1}}{Q_{n-1}}\right), \quad T = \left(\vec{t}_0\, \vec{t}_1 \ldots \vec{t}_{n-1}\right),$$

$$B\, T^T = I, \tag{33}$$

then

$$R \equiv T^T A B = \begin{pmatrix} \alpha_0 & \frac{Q_0\beta_0}{Q_1} & 0 & \cdots & 0 \\ \beta_0 & \alpha_1 & \frac{Q_1\beta_1}{Q_2} & 0 \;\cdots & 0 \\ 0 & \beta_1 & \alpha_2 & \frac{Q_2\beta_2}{Q_3} \;\cdots & 0 \\ 0 & 0 & \beta_2 & & \vdots \\ \vdots & \vdots & \vdots & \ddots & \frac{Q_{n-2}\beta_{n-2}}{Q_{n-1}} \\ 0 & 0 & 0 & \cdots & \alpha_{n-1} \end{pmatrix}. \tag{34}$$

In general, it is more easy to obtain [32] the inverse of the tridiagonal matrix *R* than A^{-1}, thus (34) implies the Lanczos expression:

$$A^{-1} = B\, R^{-1}\, T^T. \tag{35}$$

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