

A NEW LANCZOS-TYPE ALGORITHM FOR SYSTEMS OF LINEAR EQUATIONS

MUHAMMAD FAROOQ¹ AND ABDELLAH SALHI²

ABSTRACT. Lanczos-type algorithms are efficient and easy to implement. Unfortunately they breakdown frequently and well before convergence has been achieved. These algorithms are typically based on recurrence relations which involve formal orthogonal polynomials of low degree. In this paper, we consider a recurrence relation that has not been studied before and which involves a relatively higher degree polynomial. Interestingly, it leads to an algorithm that shows superior stability when compared to existing Lanczos-type algorithms. This new algorithm is derived and described. It is then compared to the best known algorithms of this type, namely A_5/B_{10} , A_8/B_{10} , as well as Arnoldi's algorithm, on a set of standard test problems. Numerical results are included.

Key words : Lanczos algorithm; Arnoldi algorithm; Systems of Linear Equations; Formal Orthogonal Polynomials

AMS SUBJECT : Primary 65F10.

1. INTRODUCTION AND BACKGROUND

The Lanczos algorithm, [28, 29, 14], is an iterative process that has been primarily designed to calculate the eigenvalues of a matrix. However, it has found a wide application in the area of Systems of Linear Equations (SLE's) where it now is a well established solver. Its attraction resides in its efficiency as it only involves vector-to-vector and matrix-to-vector products. Moreover, in exact arithmetic, it converges to the exact solution in at most n steps, where n is the dimension

¹Department of Mathematics, University of Peshawar, Khyber Pakhtunkhwa, 25120, Pakistan. Email: mfarooq@upesh.edu.pk

²Department of Mathematical Sciences, University of Essex, Wivenhoe Park, Colchester, CO4 3SQ, UK. E-mail: as@essex.ac.uk.

of the problem, [29]. While efficiency is its strong point, stability is not. Indeed, it is well known to breakdown as orthogonality of the so called Lanczos vectors, generated during the solution process, is lost. Efforts to avoid this breakdown led to a flurry of papers particularly from Brezinski and his team, [2, 5, 6, 7, 10, 12, 11, 13], and others, [4, 8, 15, 17, 20, 21, 23, 24, 31, 32, 33, 35, 38, 39].

Several Lanczos-type algorithms have been designed and among them, the famous conjugate gradient algorithm of Hestenes and Stiefel, [25], when the matrix is Hermitian and the bi-conjugate gradient algorithm of Fletcher, [22], and the algorithm of Arnoldi, [1, 36], in the general case.

Lanczos-type algorithms are commonly derived from recurrence relations typically using Formal Orthogonal Polynomials (FOP's) of low degree, [29, 6, 16, 37]. Recurrence relations using relatively higher degree FOP's have not been investigated. Here, we set out to design an algorithm that is based on such recurrence relations and FOP's, and study its properties and, in particular, its stability.

1.1. The Lanczos Process. Consider the SLE

$$A\mathbf{x} = \mathbf{b}, \quad (1)$$

where $A \in R^{n \times n}$, $\mathbf{b} \in R^n$ and $\mathbf{x} \in R^n$.

Let \mathbf{x}_0 and \mathbf{y} be two arbitrary vectors in R^n such that $\mathbf{y} \neq 0$ then Lanczos method [29] consists in constructing a sequence of vectors $\mathbf{x}_k \in R^n$ defined as follows

$$\mathbf{x}_k - \mathbf{x}_0 \in K_k(A, \mathbf{r}_0) = \text{span}(\mathbf{r}_0, A\mathbf{r}_0, \dots, A^{k-1}\mathbf{r}_0), \quad (2)$$

$$\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k \perp L_k(A^T, \mathbf{y}) = \text{span}(\mathbf{y}, A^T\mathbf{y}, \dots, A^{T^{k-1}}\mathbf{y}), \quad (3)$$

where A^T denotes the transpose of A .

Equation (2) gives,

$$\mathbf{x}_k - \mathbf{x}_0 = -\alpha_1\mathbf{r}_0 - \alpha_2A\mathbf{r}_0 - \dots - \alpha_kA^{k-1}\mathbf{r}_0. \quad (4)$$

Multiplying both sides by A and adding and subtracting \mathbf{b} on the left hand side gives

$$\mathbf{r}_k = \mathbf{r}_0 + \alpha_1\mathbf{r}_0 + \alpha_2A\mathbf{r}_0 + \dots + \alpha_kA^{k-1}\mathbf{r}_0. \quad (5)$$

If we set

$$P_k(x) = 1 + \alpha_1x + \dots + \alpha_kx,$$

then we can write from (5)

$$\mathbf{r}_k = P_k(A)\mathbf{r}_0. \quad (6)$$

From (3), the orthogonality condition gives

$$(A^{T^i} \mathbf{y}, \mathbf{r}_k) = (\mathbf{y}, A^i \mathbf{r}_k) = (\mathbf{y}, A^i \mathbf{P}_k(A) \mathbf{r}_0) = 0, \text{ for } i = 0, \dots, k-1.$$

Thus, the coefficients $\alpha_1, \dots, \alpha_k$ form a solution of SLE's,

$$\alpha_1(\mathbf{y}, A^{i+1} \mathbf{r}_0) + \dots + \alpha_k(\mathbf{y}, A^{i+k} \mathbf{r}_0) = -(\mathbf{y}, A^i \mathbf{r}_0), \text{ for } i = 0, \dots, k-1. \quad (7)$$

If the determinant of the above system is not zero then its solution exists and allows to obtain \mathbf{x}_k and \mathbf{r}_k . Obviously, in practice, solving the above system directly for increasing values of k is not feasible; k is the order of the iterate in the solution process. We shall see now how to solve this system for increasing values of k recursively, that is, if polynomials P_k can be computed recursively. Such computation is feasible, since polynomials P_k form a family of FOP's which will briefly be explained below.

1.2. Formal Orthogonal Polynomials. Define a linear functional c on the space of reel polynomials by

$$c(x^i) = c_i \text{ for } i = 0, 1, \dots$$

where

$$c_i = (A^{T^i} \mathbf{y}, \mathbf{r}_k) = (\mathbf{y}, A^i \mathbf{r}_k) \text{ for } i = 0, 1, \dots$$

Write the orthogonality condition as,

$$c(x^i P_k) = 0 \text{ for } i = 0, \dots, k-1. \quad (8)$$

The above condition shows that P_k is the polynomial of degree at most k and is a FOP with respect to the functional c , [5]. The normalization condition for these polynomials is $P_k(0) = 1$; P_k exists and is unique if the following Hankel determinant

$$H_k^{(1)} = \begin{vmatrix} c_1 & c_2 & \cdots & c_k \\ c_2 & c_3 & \cdots & c_{k+1} \\ \vdots & \vdots & & \vdots \\ c_k & c_{k+1} & \cdots & c_{2k-1} \end{vmatrix}$$

is not zero. In that case we can write $P_k(x)$ as follows.

$$P_k(x) = \frac{\begin{vmatrix} 1 & x & \cdots & x^k \\ c_0 & c_1 & \cdots & c_k \\ \vdots & \vdots & & \vdots \\ c_{k-1} & c_k & \cdots & c_{2k-1} \end{vmatrix}}{\begin{vmatrix} c_1 & \cdots & c_k \\ \vdots & & \vdots \\ c_k & \cdots & c_{2k-1} \end{vmatrix}}, \quad (9)$$

where the denominator of this polynomial is $H_k^{(1)}$, the determinant of the system (7). We assume that $\forall k$, $H_k^{(1)} \neq 0$ and therefore all the polynomials P_k exist for all k . If for some k , $H_k^{(1)} = 0$, then P_k does not exist and breakdown occurs in the algorithm, [6, 10, 11, 13, 8].

A Lanczos-type method consists in computing P_k recursively, then \mathbf{r}_k and finally \mathbf{x}_k such that $\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k$, without inverting matrix A . In exact arithmetic, this gives the solution of the system (1) in at most n steps, where n is the dimension of the SLE, [6, 12].

1.3. Notation and organization. The notation introduced by Baheux, in [2, 3], for recurrence relations with three terms is adopted here. It puts recurrence relations involving FOP's $P_k(x)$ (the polynomials of degree at most k with regard to the linear functional c) and/or FOP's $P_k^{(1)}(x)$ (the polynomials of degree at most k with regard to linear functional $c^{(1)}$, [9]) into two groups: A_i and B_j . Although relations A_i , when they exist, rarely lead to Lanczos-type algorithms on their own (the exceptions being A_4 , [2, 3], and A_{12} , [17], so far), relations B_j never lead to such algorithms for obvious reasons. It is the combination of recurrence relations A_i and B_j , denoted as A_i/B_j , when both exist, that lead to Lanczos-type algorithms. In the following we will refer to algorithms by the relation(s) that lead to them. Hence, there are, potentially, algorithms A_i and algorithms A_i/B_j , for some $i = 1, 2, \dots$ and some $j = 1, 2, \dots$

In this paper, a new algorithm based on a recurrence relation that has not been studied before, is derived. It is then compared to three other algorithms, one of which is the Arnoldi algorithm.

The rest of the paper is organized as follows. In the next section, the Lanczos-type algorithm A_8/B_{10} , [2], and the estimation of the coefficients of the recurrence relations A_8 and B_{10} used to derive it are given. Section 3 is on the estimation of the coefficients of recurrence relation

A_{12} , [17], used to derive the new algorithm of the same name. Section 4 describes the test problems and reports numerical results. Section 5 is the conclusion and further work.

2. BAHEUX ALGORITHM A_8/B_{10}

The choice of algorithm A_8/B_{10} , for comparison with our own is dictated by the fact that this is the most robust of the algorithms considered in [2, 3] on some of the problems considered here. So, outperforming this algorithm implies outperforming the rest of the algorithms considered therein.

For completeness, we recall the relevant relations between adjacent FOPs that lead to A_8/B_{10} and their coefficients estimates. These are A_8 and B_{10} . The details of algorithm A_5/B_{10} are given in [3].

2.1. Recurrence relation A_8 . Relation A_8 is

$$P_k(x) = (A_k x + B_k)P_{k-1}^{(1)}(x) + (C_k x + D_k)P_{k-1}(x), \quad (10)$$

first investigated in [2, 3]. Its coefficients are estimated as

$$B_k = 0, \quad (11)$$

$$C_k = 0, \quad (12)$$

$$D_k = 1, \quad (13)$$

and

$$A_k = -\frac{c(x^{k-1}P_{k-1}(x))}{c(x^k P_{k-1}^{(1)}(x))}. \quad (14)$$

As we know

$$\begin{cases} c(x^k P_k) = (A^{T^k} \mathbf{y}, P_k(A) \mathbf{r}_0) = (\mathbf{y}_k, \mathbf{r}_k), \\ c(x^k P_k^{(1)}) = (A^{T^k} \mathbf{y}, P_k^{(1)}(A) \mathbf{r}_0) = (\mathbf{y}_k, \mathbf{z}_k), \end{cases} \quad (15)$$

with $\mathbf{y}_k = A^T \mathbf{y}_{k-1}$ and \mathbf{z}_k is defined in (21). Using (15), equation (14) becomes

$$A_k = -\frac{(\mathbf{y}_{k-1}, \mathbf{r}_{k-1})}{(\mathbf{y}_k, \mathbf{z}_{k-1})} = -\frac{(\mathbf{y}_{k-1}, \mathbf{r}_{k-1})}{(\mathbf{y}_{k-1}, A \mathbf{z}_{k-1})}. \quad (16)$$

2.2. **Recurrence relation B_{10} .** This relation, first investigated in [2, 3], is

$$P_k^{(1)}(x) = (A_k^1 x + B_k^1) P_{k-1}^{(1)}(x) + C_k^1 P_k(x), \quad (17)$$

Its coefficients are estimated as

$$A_k^1 = 0, \quad (18)$$

$$C_k^1 a_k = 1, \quad (19)$$

where a_k is the coefficient of x^k in $P_k(x)$ defined in (10) and

$$B_k^1 = -\frac{C_k^1 c(\mathbf{y}_k, \mathbf{r}_k)}{c(\mathbf{y}_k, \mathbf{z}_{k-1})}. \quad (20)$$

Equation (17) gives

$$\mathbf{z}_k = B_k^1 \mathbf{z}_{k-1} + C_k^1 \mathbf{r}_k. \quad (21)$$

2.3. **Algorithm A_8/B_{10} .** The pseudo-code of A_8/B_{10} , due to Baheux, [2, 3], is as follows.

Algorithm 1 Algorithm A_8/B_{10}

Choose \mathbf{x}_0 and \mathbf{y} such that $\mathbf{y} \neq 0$, and ϵ arbitrarily small and positive.

Set $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$,

$\mathbf{z}_0 = \mathbf{r}_0$,

$\mathbf{y}_0 = \mathbf{y}$,

for $k = 0, 1, 2, \dots$, **do**

$$A_{k+1} = -\frac{(\mathbf{y}_k, \mathbf{r}_k)}{(\mathbf{y}_k, A\mathbf{z}_k)},$$

$$\mathbf{r}_{k+1} = \mathbf{r}_k + A_{k+1} A\mathbf{z}_k,$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k - A_{k+1} \mathbf{z}_k.$$

if $\|\mathbf{r}_{k+1}\| \geq \epsilon$, **then**

$$\mathbf{y}_{k+1} = A^T \mathbf{y}_k,$$

$$C_{k+1}^1 = \frac{1}{A_{k+1}},$$

$$B_{k+1}^1 = -\frac{C_{k+1}^1 (\mathbf{y}_{k+1}, \mathbf{r}_{k+1})}{(\mathbf{y}_k, A\mathbf{z}_k)},$$

$$\mathbf{z}_{k+1} = B_{k+1}^1 \mathbf{z}_k + C_{k+1}^1 \mathbf{r}_{k+1}.$$

else

Stop; solution found.

end if

end for

3. A NEW LANCZOS-TYPE ALGORITHM

In the following, a new recurrence relation which leads to a new variant of the Lanczos algorithm is considered.

3.1. Recurrence relation A_{12} . Consider the following recurrence relation, [17, 19]

$$P_k(x) = A_k[(x^2 + B_kx + C_k)P_{k-2}(x) + (D_kx^3 + E_kx^2 + F_kx + G_k)P_{k-3}(x)], \quad (22)$$

for $k \geq 3$, where $A_k, B_k, C_k, D_k, E_k, F_k$ and G_k are constants to be determined using the normalization condition $P_k(0) = 1$ and the orthogonality conditions $c(x^i P_k) = 0, \forall i = 0, \dots, k-1$, x^i being a monic polynomial of exact degree i . To find these coefficients, we proceed as follows. Since $\forall k, P_k(0) = 1$, equation (22) gives

$$1 = A_k[C_k + G_k].$$

Multiplying both sides of (22) by x^i and then applying the linear functional c , we get

$$c(x^i P_k) = A_k\{c(x^{i+2} P_{k-2}) + B_k c(x^{i+1} P_{k-2}) + C_k c(x^i P_{k-2}) + D_k c(x^{i+3} P_{k-3}) + E_k c(x^{i+2} P_{k-3}) + F_k c(x^{i+1} P_{k-3}) + G_k c(x^i P_{k-3})\}. \quad (23)$$

Equation (23) is always true for $i = 0, \dots, k-7$.

For $i = k-6$, we have

$$0 = D_k c(x^{k-3} P_{k-3}).$$

Since $c(x^{k-3} P_{k-3}) \neq 0$, we have

$$D_k = 0.$$

For $i = k-5$, we get

$$0 = E_k c(x^{k-3} P_{k-3}).$$

But $c(x^{k-3} P_{k-3}) \neq 0$; therefore

$$E_k = 0.$$

For $i = k-4$, (23) gives

$$F_k = -\frac{c(x^{k-2} P_{k-2})}{c(x^{k-3} P_{k-3})}. \quad (24)$$

For $i = k - 3$, $i = k - 2$ and $i = k - 1$ we get the following equations respectively

$$B_k c(x^{k-2} P_{k-2}) + G_k c(x^{k-3} P_{k-3}) = -c(x^{k-1} P_{k-2}) - F_k c(x^{k-2} P_{k-3}), \quad (25)$$

$$\begin{aligned} B_k c(x^{k-1} P_{k-2}) + C_k c(x^{k-2} P_{k-2}) + G_k c(x^{k-2} P_{k-3}) \\ = -c(x^k P_{k-2}) - F_k c(x^{k-1} P_{k-3}), \end{aligned} \quad (26)$$

and

$$\begin{aligned} B_k c(x^k P_{k-2}) + C_k c(x^{k-1} P_{k-2}) + G_k c(x^{k-1} P_{k-3}) \\ = -c(x^{k+1} P_{k-2}) - F_k c(x^k P_{k-3}). \end{aligned} \quad (27)$$

Let a_{11} , a_{12} , a_{13} , a_{21} , a_{22} , a_{23} , a_{31} , a_{32} , and a_{33} be the coefficients of B_k , C_k and G_k in equations (25), (26) and (27) respectively and let b_1 , b_2 and b_3 be the corresponding right sides of these equations. If Δ_k represents the determinant of the coefficients matrix of the above mentioned system of equations then, we have

$$a_{11} = c(x^{k-2} P_{k-2}), \quad a_{12} = 0, \quad a_{13} = c(x^{k-3} P_{k-3}),$$

$$a_{21} = c(x^{k-1} P_{k-2}), \quad a_{22} = c(x^{k-2} P_{k-2}), \quad a_{23} = c(x^{k-2} P_{k-3}),$$

$$a_{31} = c(x^k P_{k-2}), \quad a_{32} = c(x^{k-1} P_{k-2}), \quad a_{33} = c(x^{k-1} P_{k-3}),$$

$$b_1 = -c(x^{k-1} P_{k-2}) - F_k c(x^{k-2} P_{k-3}) = -a_{21} - F_k a_{23},$$

$$b_2 = -c(x^k P_{k-2}) - F_k c(x^{k-1} P_{k-3}) = -a_{31} - F_k a_{33},$$

$$b_3 = -c(x^{k+1} P_{k-2}) - F_k c(x^k P_{k-3}) = -s - F_k t, \quad \text{where } s = c(x^{k+1} P_{k-2}) \text{ and } t = c(x^k P_{k-3}).$$

Therefore, equations (25), (26) and (27) can be written as

$$a_{11} B_k + 0 C_k + a_{13} G_k = b_1, \quad (28)$$

$$a_{21} B_k + a_{22} C_k + a_{23} G_k = b_2, \quad (29)$$

$$a_{31} B_k + a_{32} C_k + a_{33} G_k = b_3. \quad (30)$$

To solve for B_k , C_k and G_k , Cramer's rule requires

$$\Delta_k = a_{11}(a_{22}a_{33} - a_{32}a_{23}) + a_{13}(a_{21}a_{32} - a_{31}a_{22}).$$

If $\Delta_k \neq 0$, then

$$B_k = \frac{b_1(a_{22}a_{33} - a_{32}a_{23}) + a_{13}(b_2a_{32} - b_3a_{22})}{\Delta_k}, \quad (31)$$

$$G_k = \frac{b_1 - a_{11}B_k}{a_{13}}, \quad (32)$$

$$C_k = \frac{b_2 - a_{21}B_k - a_{23}G_k}{a_{22}}, \quad (33)$$

and

$$1 = A_k[C_k + G_k]. \quad (34)$$

With all the necessary coefficients now determined, the expression of the polynomials $P_k(x)$ becomes

$$P_k(x) = A_k\{(x^2 + B_kx + C_k)P_{k-2}(x) + (F_kx + G_k)P_{k-3}(x)\}. \quad (35)$$

Let us now use the relation (35) to compute $P_k(x)$, necessary for the computation of the residual $\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k = P_k(A)\mathbf{r}_0$ and the corresponding vector \mathbf{x}_k .

Assume that P_k has exact degree k and the 3-term recurrence relationship (35) holds. To move to the Krylov space, replace x by A and multiply both side of (35) by \mathbf{r}_0 to get,

$$P_k(A)\mathbf{r}_0 = A_k[(A^2 + B_kA + C_kI)P_{k-2}(A)\mathbf{r}_0 + (F_kA + G_kI)P_{k-3}(A)\mathbf{r}_0]. \quad (36)$$

Using equation (6), gives

$$\mathbf{r}_k = A_k\{(A^2 + B_kA + C_kI)\mathbf{r}_{k-2} + (F_kA + G_kI)\mathbf{r}_{k-3}\}. \quad (37)$$

And using $\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k$, gives

$$\mathbf{x}_k = A_k\{C_k\mathbf{x}_{k-2} + G_k\mathbf{x}_{k-3} - (A\mathbf{r}_{k-2} + B_k\mathbf{r}_{k-2} + F_k\mathbf{r}_{k-3})\}, \quad (38)$$

with F_k as in equation (24). Using (15), F_k can be written as

$$F_k = -\frac{(\mathbf{y}_{k-2}, \mathbf{r}_{k-2})}{(\mathbf{y}_{k-3}, \mathbf{r}_{k-3})}.$$

Condition (15) can be used equally to rewrite the expressions of a_{11} , through a_{33} , b_1 to b_3 as follows.

$$a_{11} = (\mathbf{y}_{k-2}, \mathbf{r}_{k-2}), \quad a_{12} = 0, \quad a_{13} = (\mathbf{y}_{k-3}, \mathbf{r}_{k-3}),$$

$$a_{21} = (\mathbf{y}_{k-1}, \mathbf{r}_{k-2}), \quad a_{22} = (\mathbf{y}_{k-2}, \mathbf{r}_{k-2}), \quad a_{23} = (\mathbf{y}_{k-2}, \mathbf{r}_{k-3}),$$

$$a_{31} = (\mathbf{y}_k, \mathbf{r}_{k-2}), \quad a_{32} = (\mathbf{y}_{k-1}, \mathbf{r}_{k-2}), \quad a_{33} = (\mathbf{y}_{k-1}, \mathbf{r}_{k-3}),$$

$$b_1 = -a_{21} - F_k a_{23}, \quad b_2 = -a_{31} - F_k a_{33}, \quad b_3 = -s - F_k t,$$

where $s = (\mathbf{y}_{k+1}, \mathbf{r}_{k-2})$ and $t = (\mathbf{y}_k, \mathbf{r}_{k-3})$.

These parameters allow the explicit computation of B_k , G_k , C_k , and A_k as is given by equations 31, 32, 33 and 34 respectively. Equations (37) and (38) define the new Lanczos-type algorithm.

Now, since all previous formulae are only valid for $k \geq 3$, it is necessary to find the expressions of the polynomials of degrees 1 and 2. From (9), we can write

$$P_1(x) = \frac{\begin{vmatrix} 1 & x \\ c_0 & c_1 \end{vmatrix}}{c_1},$$

$$P_1(x) = 1 - \frac{c_0}{c_1}x,$$

$\mathbf{r}_1 = \mathbf{r}_0 - \frac{c_0}{c_1}A\mathbf{r}_0$, and $\mathbf{x}_1 = \mathbf{x}_0 + \frac{c_0}{c_1}\mathbf{r}_0$, where $c_i = (\mathbf{y}, A^i\mathbf{r}_0)$.

Using (9) again, we can write

$$P_2(x) = \frac{\begin{vmatrix} 1 & x & x^2 \\ c_0 & c_1 & c_2 \\ c_1 & c_2 & c_3 \end{vmatrix}}{\begin{vmatrix} c_1 & c_2 \\ c_2 & c_3 \end{vmatrix}},$$

$$P_2(x) = 1 - \frac{c_0c_3 - c_1c_2}{c_1c_3 - c_2^2}x + \frac{c_0c_2 - c_1^2}{c_1c_3 - c_2^2}x^2,$$

$\mathbf{r}_2 = \mathbf{r}_0 - \alpha A\mathbf{r}_0 + \beta A^2\mathbf{r}_0$, and $\mathbf{x}_2 = \mathbf{x}_0 + \alpha\mathbf{r}_0 - \beta A\mathbf{r}_0$, where $\alpha = \frac{c_0c_3 - c_1c_2}{\delta}$, $\beta = \frac{c_0c_2 - c_1^2}{\delta}$ and $\delta = c_1c_3 - c_2^2$.

3.2. Algorithm A_{12} . Putting together the various steps given in the above section, the new algorithm can be described as follows.

Algorithm 2 Algorithm A_{12}

Choose \mathbf{x}_0 and \mathbf{y} such that $\mathbf{y} \neq 0$, and choose ϵ arbitrarily small and positive.

Set $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$, $\mathbf{y}_0 = \mathbf{y}$, $\mathbf{p} = A\mathbf{r}_0$, $\mathbf{p}_1 = A\mathbf{p}$, $c_0 = (\mathbf{y}, \mathbf{r}_0)$,

$c_1 = (\mathbf{y}, \mathbf{p})$, $c_2 = (\mathbf{y}, \mathbf{p}_1)$, $c_3 = (\mathbf{y}, A\mathbf{p}_1)$, $\delta = c_1c_3 - c_2^2$,

$\alpha = \frac{c_0c_3 - c_1c_2}{\delta}$, $\beta = \frac{c_0c_2 - c_1^2}{\delta}$,

$\mathbf{r}_1 = \mathbf{r}_0 - \frac{c_0}{c_1}\mathbf{p}$, $\mathbf{x}_1 = \mathbf{x}_0 + \frac{c_0}{c_1}\mathbf{r}_0$,

$\mathbf{r}_2 = \mathbf{r}_0 - \alpha\mathbf{p} + \beta\mathbf{p}_1$, $\mathbf{x}_2 = \mathbf{x}_0 + \alpha\mathbf{r}_0 - \beta\mathbf{p}$,

$\mathbf{y}_1 = A^T\mathbf{y}_0$, $\mathbf{y}_2 = A^T\mathbf{y}_1$, $\mathbf{y}_3 = A^T\mathbf{y}_2$, $k = 3$.

while $\|r_k\| \geq \epsilon$ **do**

$\mathbf{y}_{k+1} = A^T\mathbf{y}_k$, $\mathbf{q}_1 = A\mathbf{r}_{k-1}$, $\mathbf{q}_2 = A\mathbf{q}_1$, $\mathbf{q}_3 = A\mathbf{r}_{k-2}$,

$a_{11} = (\mathbf{y}_{k-2}, \mathbf{r}_{k-2})$, $a_{13} = (\mathbf{y}_{k-3}, \mathbf{r}_{k-3})$, $a_{21} = (\mathbf{y}_{k-1}, \mathbf{r}_{k-2})$, $a_{22} = a_{11}$,

$a_{23} = (\mathbf{y}_{k-2}, \mathbf{r}_{k-3})$, $a_{31} = (\mathbf{y}_k, \mathbf{r}_{k-2})$, $a_{32} = a_{21}$, $a_{33} = (\mathbf{y}_{k-1}, \mathbf{r}_{k-3})$,

$s = (\mathbf{y}_{k+1}, \mathbf{r}_{k-2})$, $t = (\mathbf{y}_k, \mathbf{r}_{k-3})$, $F_k = -\frac{a_{11}}{a_{13}}$,

$b_1 = -a_{21} - a_{23}F_k$, $b_2 = -a_{31} - a_{33}F_k$, $b_3 = -s - tF_k$,

$\Delta_k = a_{11}(a_{22}a_{33} - a_{32}a_{23}) + a_{13}(a_{21}a_{32} - a_{31}a_{22})$,

$B_k = \frac{b_1(a_{22}a_{33} - a_{32}a_{23}) + a_{13}(b_2a_{32} - b_3a_{22})}{\Delta_k}$,

$G_k = \frac{b_1 - a_{11}B_k}{a_{13}}$,

$C_k = \frac{b_2 - a_{21}B_k - a_{23}G_k}{a_{22}}$,

$A_k = \frac{1}{C_k + G_k}$,

$\mathbf{r}_k = A_k\{\mathbf{q}_2 + B_k\mathbf{q}_1 + C_k\mathbf{r}_{k-2} + F_k\mathbf{q}_3 + G_k\mathbf{r}_{k-3}\}$,

$\mathbf{x}_k = A_k\{C_k\mathbf{x}_{k-2} + G_k\mathbf{x}_{k-3} - (\mathbf{q}_1 + B_k\mathbf{r}_{k-2} + F_k\mathbf{r}_{k-3})\}$,

$k = k + 1$.

end while

Stop; solution found.

4. NUMERICAL RESULTS

A_{12} , [17], the algorithm described in the above section, has been tested against algorithms A_5/B_{10} and A_8/B_{10} , the best algorithms according to [3, 2], as well as against the established Arnoldi algorithm, [1, 36].

4.1. Test problems I. The test problems considered here arise in the 5-point discretisation of the operator $\frac{-d^2}{dx^2} - \frac{d^2}{dy^2} + \gamma \frac{d}{dx}$ on a rectangular region. Comparative results on instances of the following problem ranging from dimension 10 to 100 for parameter δ taking values 0.0 and 0.2 respectively, are recorded in Table 1 and Table 2.

$$A = \begin{pmatrix} B & -I & \cdots & \cdots & 0 \\ -I & B & -I & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & -I & B & -I \\ 0 & \cdots & \cdots & -I & B \end{pmatrix}, \text{ with } B = \begin{pmatrix} 4 & \alpha & \cdots & \cdots & 0 \\ \beta & 4 & \alpha & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \beta & 4 & \alpha \\ 0 & \cdots & & \beta & 4 \end{pmatrix}.$$

and $\alpha = -1 + \delta$, and $\beta = -1 - \delta$. The right-hand side is $\mathbf{b} = A\mathbf{x}$, where $\mathbf{x} = (1, 1, \dots, 1)^T$, is the solution of the system. The dimension of B is 10.

TABLE 1. Experimental results for problems when $\delta = 0$

n	Arnoldi		A_5/B_{10}		A_8/B_{10}		A_{12}	
	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)
10	$1.2514E^{-10}$	0.001450	$2.2940E^{-13}$	0.001892	$1.7704E^{-13}$	0.002770	$4.9623E^{-13}$	0.002819
20	$1.7733E^{-11}$	0.002207	$2.5256E^{-14}$	0.001842	$1.7489E^{-13}$	0.002654	$1.7536E^{-13}$	0.002904
30	$1.2990E^{-14}$	0.003602	$3.9026E^{-09}$	0.002220	$4.9472E^{-09}$	0.003179	$5.4705E^{-08}$	0.003370
40	$3.5434E^{-11}$	0.006071	$1.4770E^{-10}$	0.002416	$8.4658E^{-10}$	0.003095	$1.4776E^{-08}$	0.003526
50	$6.1827E^{-08}$	0.008870	$1.9959E^{-06}$	0.002962	$1.3598E^{-06}$	0.003696	$4.7994E^{-06}$	0.003980
60	$2.9843E^{-14}$	0.012282	$9.1910E^{-06}$	0.003001	$3.7470E^{-06}$	0.003776	$5.0010E^{-06}$	0.004354
70	$4.2642E^{-13}$	0.017151	$4.9035E^{-06}$	0.003622	$4.2579E^{-06}$	0.004194	$1.3781E^{-06}$	0.005658
80	$5.0951E^{-08}$	0.021938	$4.4311E^{-06}$	0.004498	$7.7199E^{-06}$	0.005504	$7.5581E^{-06}$	0.005271
90	$9.6960E^{-13}$	0.029083	<i>NaN</i>		$8.5560E^{-06}$	0.007900	$3.7301E^{-06}$	0.006541
100	$1.1397E^{-13}$	0.036462	$1.1889E^{-06}$	0.003849	$3.1695E^{-06}$	0.004499	$8.9530E^{-07}$	0.005084

TABLE 2. Experimental results for problems when $\delta = 0.2$

n	Arnoldi		A_5/B_{10}		A_8/B_{10}		A_{12}	
	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)
10	$2.3499E^{-15}$	0.001377	$5.2347E^{-04}$	0.002339	$5.2347E^{-04}$	0.002948	$5.2347E^{-04}$	0.003231
20	$5.6622E^{-11}$	0.002149	$4.1778E^{-11}$	0.001842	$5.8526E^{-11}$	0.003090	$6.3915E^{-10}$	0.003372
30	$6.8771E^{-15}$	0.003573	$8.9881E^{-04}$	0.002220	$8.9880E^{-04}$	0.003580	$8.9880E^{-04}$	0.003847
40	$1.8106E^{-10}$	0.006137	$8.7583E^{-04}$	0.002830	$9.3988E^{-04}$	0.003620	$9.1261E^{-04}$	0.003977
50	$3.5345E^{-08}$	0.008552	$6.2669E^{-04}$	0.003360	$5.7269E^{-04}$	0.004055	$2.5040E^{-04}$	0.004964
60	$2.8757E^{-13}$	0.012544	$6.3670E^{-04}$	0.003877	$8.4915E^{-04}$	0.004885	$7.3489E^{-04}$	0.005345
70	$4.2552E^{-13}$	0.017352	$8.5670E^{-04}$	0.003902	$7.0703E^{-04}$	0.006158	$9.9086E^{-04}$	0.005052
80	$1.7785E^{-04}$	0.021629	<i>NaN</i>		<i>NaN</i>		$6.5602E^{-04}$	0.012131
90	$1.4837E^{-04}$	0.029332	<i>NaN</i>		$7.5451E^{-04}$	0.011230	$9.5294E^{-04}$	0.011842
100	$5.8942E^{-13}$	0.037067	<i>NaN</i>		<i>NaN</i>		$9.9710E^{-04}$	0.018899

4.2. **Test problems II.** The coefficient matrix here is taken as the Hilbert matrix, i.e. $A = \text{hilb}(n)$, where $\text{hilb}(n)$ is a Matlab function,

n being the dimension of A . The right-hand side \mathbf{b} and the solution \mathbf{x} , are defined in the same way as in test problems I. The Hilbert matrix is notoriously ill-conditioned. Ill-conditioned systems of linear equations are notoriously difficult to solve to any useful accuracy, [18, 27, 34]

TABLE 3. Experimental results when A is a Hilbert matrix.

n	Arnoldi		A_5/B_{10}		A_8/B_{10}		A_{12}	
	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)	$\ r_k\ $	t(sec)
10	$3.2101E^{-15}$	0.002364	$4.4809E^{-06}$	0.001945	$4.4809E^{-06}$	0.002834	$4.4809E^{-06}$	0.002706
20	$2.2288E^{-15}$	0.003285	$9.6002E^{-05}$	0.001772	$9.6002E^{-05}$	0.002839	$9.6002E^{-05}$	0.002787
30	$3.8953E^{-15}$	0.004148	$1.3341E^{-05}$	0.001929	$1.3376E^{-05}$	0.003050	$1.3340E^{-05}$	0.002791
40	$3.2251E^{-14}$	0.005521	$3.8228E^{-05}$	0.001880	$3.8276E^{-05}$	0.003327	$3.8229E^{-05}$	0.002772
50	$2.8673E^{-15}$	0.007068	$7.9457E^{-05}$	0.001997	$7.9463E^{-05}$	0.003475	$7.9457E^{-05}$	0.003334

All algorithms have been implemented in Matlab version 7.8.0 and run on a PC, under Microsoft Windows XP Professional Operating System, with 3.2GB RAM, and 2.40 GHz Intel(R) Core(TM) 2 CPU 6600. The problems are solved as dense problems, i.e. no sparsity has been exploited. The results point to the Arnoldi algorithm being the most robust overall, but also the slowest overall. Algorithms A_5/B_{10} and A_8/B_{10} are the fastest overall, but the least robust overall; in fact they have failed to solve some problems in high dimension due to breakdown, of course, which is endemic in Lanczos-type algorithms. Algorithm A_{12} , like Arnoldi, solved all problems but faster and not as accurately. It is also more robust than A_5/B_{10} and A_8/B_{10} overall, but slower than both of them overall. Its lower speed compared to that of A_5/B_{10} and A_8/B_{10} is expected since the recurrence relation A_{12} involves more coefficients than both recurrence relations A_5/B_{10} and A_8/B_{10} . Note that on the Hilbert-type problems, Table 3, the algorithms could not cope with dimensions higher than 50. Arnoldi is again the most stable overall and the slowest as the dimension grows. The other three algorithms have similar performances.

5. CONCLUSION AND FURTHER WORK

The way Lanczos-type algorithms are derived using recurrence relations involving FOP's means that many such algorithms can be created, each based on a different set of relations. The choice of recurrence relations to use is dictated by the degree of FOP's to be involved; high degrees mean a large number of coefficients have to be calculated in the

concerned Lanczos process. This, consequently, dictates the computational complexity of the resulting Lanczos-type algorithm. However, it is well known, [26, 30], that computational complexity does not always imply efficiency, or indeed robustness. Moreover, robustness and accuracy are often more important. It is therefore worthwhile to look beyond complexity issues sometimes, like we did here.

In this paper we have shown that, indeed, there are recurrence relations worth exploring since they lead to more robust algorithms. As a result, a new Lanczos-type algorithm, A_{12} has been designed. The numerical performance of this algorithm is compared to that of two existing Lanczos-type algorithms, which were found to be the best among a number of Lanczos-type algorithms, [2, 3], on the same set of problems as considered here. It is also compared to the well established Arnoldi algorithm. It is interesting to find that algorithm A_{12} is overall more robust than A_5/B_{10} and A_8/B_{10} and faster than Arnoldi's. This makes it occupy, at least on the set of problems used here and elsewhere, a happy medium position. It is therefore the ideal candidate for time-limited applications which do not require high accuracy.

REFERENCES

- [1] W. E. Arnoldi. The principal of minimized iterations in the solution of the matrix eigenvalue problem. *Quarterly of Applied Mathematics*, 9 (1951):17–29.
- [2] C. Baheux. New Implementations of Lanczos Method. *Journal of Computational and Applied Mathematics*, 57 (1995):3–15.
- [3] C. Baheux. *Algorithmes d'implémentation de la méthode de Lanczos*. PhD thesis, University of Lille 1, France, 1994.
- [4] A. Björck, T. Elfving, and Z. Strakos. Stability of Conjugate Gradient and Lanczos Methods for Linear Least Squares Problems. *SIAM Journal of Matrix Analysis and Application*, 19 (1998):720–736.
- [5] C. Brezinski. *Padé-Type Approximation and General Orthogonal Polynomials, Internat. Ser. Numer. Math. 50*. Birkhäuser, Basel, 1980.
- [6] C. Brezinski and H. Sadok. Lanczos-type algorithms for solving systems of linear equations. *Applied Numerical Mathematics*, 11 (1993):443–473.
- [7] C. Brezinski and M. R. Zaglia. Hybrid procedures for solving linear systems. *Numerische Mathematik*, 67 (1994):1–19.
- [8] C. Brezinski and M. R. Zaglia. A New Presentation of Orthogonal Polynomials with Applications to their Computation. *Numerical Algorithms*, 1 (1991):207–222.
- [9] C. Brezinski, M. R. Zaglia, and H. Sadok. Avoiding breakdown and near-breakdown in Lanczos type algorithms. *Numerical Algorithms*, 1 (1991):261–284.
- [10] C. Brezinski, M. R. Zaglia, and H. Sadok. A Breakdown-free Lanczos type algorithm for solving linear systems. *Numerische Mathematik*, 63 (1992):29–38.

- [11] C. Brezinski, M. R. Zaglia, and H. Sadok. The matrix and polynomial approaches to Lanczos-type algorithms. *Journal of Computational and Applied Mathematics*, 123 (2000):241–260.
- [12] C. Brezinski, M. R. Zaglia, and H. Sadok. New look-ahead Lanczos-type algorithms for linear systems. *Numerische Mathematik*, 83 (1999):53–85.
- [13] C. Brezinski, M. R. Zaglia, and H. Sadok. A review of formal orthogonality in Lanczos-based methods. *Journal of Computational and Applied Mathematics*, 140 (2002):81–98.
- [14] C. G. Broyden and M. T. Vespucchi. *Krylov Solvers For Linear Algebraic Systems*. Elsevier, Amsterdam, The Netherlands, 2004.
- [15] D. Calvetti, L. Reichel, F. Sgallari, and G. Spaletta. A Regularizing Lanczos iteration method for underdetermined linear systems. *Journal of Computational and Applied Mathematics*, 115 (2000):101–120.
- [16] A. Draux. *Polynômes Orthogonaux Formels. Application, LNM 974*. Springer-Verlag, Berlin, 1983.
- [17] M. Farooq. *New Lanczos-type Algorithms and their Implementation*. PhD thesis, University of Essex, UK, 2011. <http://serlib0.essex.ac.uk/record=b1754556>.
- [18] M. Farooq and A. Salhi. Improving the solvability of ill-conditioned systems of linear equations by reducing the condition number of their matrices. *J. Korean Math. Soc.*, 48 (5) (2011):939–952. <http://dx.doi.org/10.4134/JKMS.2011.48.5.939>.
- [19] M. Farooq and A. Salhi. New Recurrence Relationships Between Orthogonal Polynomials Which Lead to New Lanczos-type Algorithms. *Journal of Prime Research in Mathematics*, 8 (2012):61–75. <http://www.sms.edu.pk/journals/jprm/jprmvol8/09.pdf>.
- [20] M. Farooq and A. Salhi. A Preemptive Restarting Approach to Beating the Inherent Instability of Lanczos-type Algorithms. *Iranian Journal of Science and Technology, Transaction A: Science*, 37 (3.1) (2013):349–358. http://ijsts.shirazu.ac.ir/?_action=articleInfo&article=1634&vol=142.
- [21] M. Farooq and A. Salhi. A Switching Approach to Avoid Breakdown in Lanczos-type Algorithms. *Applied Mathematics and Information Sciences*, 8 (5) (2014):2161–2169. <http://naturalspublishing.com/ContIss.asp?IssID=190>.
- [22] R. Fletcher. Conjugate gradient methods for indefinite systems. In G. Alistair Watson, editor, *Numerical Analysis*, volume 506 of *Lecture Notes in Mathematics*, pages 73–89. Springer Berlin Heidelberg, 1976.
- [23] A. Greenbaum. *Iterative Methods for Solving Linear System*. Society for Industrial and Applied Mathematics, Philadelphia, 1997.
- [24] A. El Guennouni. A unified approach to some strategies for the treatment of breakdown in Lanczos-type algorithms. *Applicationes Mathematicae*, 26 (1999):477–488.
- [25] M.R. Hestenes and E. Stiefel. Methods of conjugate gradients for solving linear systems. *Journal of the National Bureau of Standards*, 49 (1952):409–436.

- [26] L. G. Khachyan. A polynomial algorithm in linear programming. *Soviet Mathematics Doklady (translated)*, 20 (1979):191–194.
- [27] H. J. Kim, K. Choi, H. B. Lee, H. K. Jung, and S. Y. Hahn. A new algorithm for solving ill-conditioned linear system. *IEEE Transactions on Magnetics*, 32(3) (1996):1373–1376.
- [28] C. Lanczos. An Iteration Method for the Solution of the Eigenvalue Problem of Linear Differential and Integral Operators. *Journal of Research of the National Bureau of Standards*, 45 (1950):255–282.
- [29] C. Lanczos. Solution of systems of linear equations by minimized iteration. *Journal of the National Bureau of Standards*, 49 (1952):33–53.
- [30] L. Lovasz. The Ellipsoid Algorithm: Better or Worse than the Simplex? *Mathematical Intelligencer*, 2 (1980):141–146.
- [31] G. Meurant. *The Lanczos and conjugate gradient algorithms, From Theory to Finite Precision Computations*. SIAM, Philadelphia, 2006.
- [32] B. N. Parlett and D. S. Scott. The Lanczos Algorithm With Selective Orthogonalization. *Mathematics of Computation*, 33 (1979):217–238.
- [33] B. N. Parlett, D. R. Taylor, and Z. A. Liu. A Look-Ahead Lanczos Algorithm for Unsymmetric Matrices. *Mathematics of Computation*, 44 (1985):105–124.
- [34] J. R. Rice. *Matrix Computations and Mathematical Software*. McGraw-Hill, New York, 1981.
- [35] Y. Saad. On the Lanczos method for solving linear system with several right-hand sides. *Mathematics of Computation*, 48 (1987):651–662.
- [36] Y. Saad. *Iterative methods for sparse linear systems*. SIAM, Philadelphia, 2003.
- [37] G. Szegő. *Orthogonal Polynomials*. American Mathematical Society, Providence, Rhode Island, 1939.
- [38] H. A. Van der Vorst. An iterative solution method for solving $f(A)\mathbf{x}=\mathbf{b}$, using Krylov subspace information obtained for the symmetric positive definite matrix A . *Journal of Computational and Applied Mathematics*, 18(2) (1987):249–263.
- [39] Q. Ye. A Breakdown-Free Variation of the Nonsymmetric Lanczos Algorithms. *Mathematics of Computation*, 62 (1994):179–207.