APPLICATIONES MATHEMATICAE
26,1 (1999), pp. 33–62

E. H. AYACHOUR (Lille)

AVOIDING LOOK-AHEAD IN THE LANCZOS METHOD AND PADÉ APPROXIMATION

Abstract. In the non-normal case, it is possible to use various look-ahead strategies for computing the elements of a family of regular orthogonal polynomials. These strategies consist in jumping over non-existing and singular orthogonal polynomials by solving triangular linear systems. We show how to avoid them by using a new method called ALA (Avoiding Look-Ahead), for which we give three principal implementations. The application of ALA to Padé approximation, extrapolation methods and Lanczos method for solving systems of linear equations is discussed.

1. Introduction. A Hankel system comes up implicitly in the Lanczos method, in Padé approximation and in extrapolation methods. The principal submatrices of a Hankel matrix are Hankel matrices of linear systems which are solved by using orthogonal polynomials. It is well known that these orthogonal polynomials satisfy a three-term recurrence relation. When some of them are singular, a breakdown (or a so-called *true breakdown* [8]) problem occurs in this recurrence relation. To avoid such a problem, Draux [16] has shown how to compute regular orthogonal polynomials by using look-ahead strategies. A look-ahead strategy consists in jumping over the non-existing orthogonal polynomials. Draux and Van Ingelandt applied this technique to Padé approximation in [17] where they give algorithms which allow moving in the Padé table along a diagonal, a row, a staircase consisting of two adjacent diagonals and a sawtooth consisting of two adjacent rows. Gutknecht and Hochbruck used the Levinson–Schur type recurrences with look-ahead strategies for computing Padé approximants [23, 22]. Brezinski, Redivo Zaglia and Sadok have applied these look-ahead strategies to the

1991 *Mathematics Subject Classification*: 42C05, 41A21, 65F10, 65B05, 65B10.
Key words and phrases: orthogonal and biorthogonal polynomials, Lanczos method, Padé approximation, extrapolation methods.

Lanczos method [10, 12]. These strategies have also been applied to QMR by Freund, Gutknecht and Nachtigal [18, 25].

In this paper, we will show how to substitute new intermediate polynomials instead of look-ahead strategies. These intermediate polynomials are biorthogonal and satisfy a simple three-term recurrence relation. In addition, they can be considered as an alternative for orthogonal polynomials which are singular or non-existent.

For a given integer $n \in \mathbb{Z}$, we consider the linear functional $C^{(n)}$ defined on the space $\mathbb{C}[X]$ of polynomials by $C^{(n)}(x^i) = c_{n+i}$. By convention, we set $c_i = 0$ when $i < 0$. We denote by $H_k^{\theta_n}$ the following determinant:

$$H_k^{\theta_n} = \begin{vmatrix} c_{\theta_n(0)+n} & c_{\theta_n(0)+n+1} & \cdots & c_{\theta_n(0)+n+k-1} \\ c_{\theta_n(1)+n} & c_{\theta_n(1)+n+1} & \cdots & c_{\theta_n(1)+n+k-1} \\ \vdots & \vdots & & \vdots \\ c_{\theta_n(k-1)+n} & c_{\theta_n(k-1)+n+1} & \cdots & c_{\theta_n(k-1)+n+k-1} \end{vmatrix}$$

where θ_n is a permutation of $\mathbb{N}$ recursively defined by associating with every $j \in \mathbb{N}$ the smallest integer $\theta_n(j)$ satisfying $H_{j+1}^{\theta_n} \neq 0$. So, $\theta_n(0) = i_0$ if i_0 is the smallest integer such that $c_{i_0+n} \neq 0$, $\theta_n(1)$ is the smallest integer such that $H_2^{\theta_n} \neq 0$, and so on.

2. Orthogonality. For a fixed integer n, let $\{P_i^{(n)}\}_i$ be the family of orthogonal polynomials such that, for all i, $P_i^{(n)}$ has degree i and

$$C^{(n)}(x^j P_i^{(n)}(x)) = 0 \qquad \text{for } j = 0, 1, \ldots, i-1. \tag{1}$$

For every i and n, if the set of all solutions of (1) is a subspace of dimension 1, then $P_i^{(n)}$ is called *regular*. The explicit expression of each orthogonal polynomial $P_i^{(n)}$ is given in [8]:

$$P_i^{(n)}(x) = \begin{vmatrix} c_n & c_{n+1} & \cdots & c_{n+i} \\ c_{n+1} & c_{n+2} & \cdots & c_{n+i+1} \\ \vdots & \vdots & & \vdots \\ c_{n+i-1} & c_{n+i} & \cdots & c_{n+2i-1} \\ 1 & x & \cdots & x^i \end{vmatrix} \Big/ d_i^{(n)},$$

where $d_i^{(n)}$ is the determinant

$$\begin{vmatrix} c_n & c_{n+1} & \cdots & c_{n+i} \\ c_{n+1} & c_{n+2} & \cdots & c_{n+i+1} \\ \vdots & \vdots & & \vdots \\ c_{n+i-1} & c_{n+i} & \cdots & c_{n+2i-1} \\ a_0^{n,i} & a_1^{n,i} & \cdots & a_i^{n,i} \end{vmatrix}.$$

Each choice of the coefficients $\{a_j^{n,i}\}_{j=0,\ldots,i}$ corresponds to a different normalization of the orthogonal polynomial $P_i^{(n)}$. In the sequel, we will examine three normalizations:

1. In Padé approximation, we choose $a_0^{n,i} = a_1^{n,i} = \ldots = a_{i-1}^{n,i} = 0$ and $a_i^{n,i} = 1$. Thus $P_i^{(n)}$ is a monic polynomial of degree i.

2. For the Lanczos method, we set $a_1^{n,i} = a_2^{n,i} = \ldots = a_i^{n,i} = 0$ and $a_0^{n,i} = 1$, which is equivalent to the condition $P_i^{(n)}(0) = 1$.

3. In extrapolation methods, we choose $a_0^{n,i} = a_1^{n,i} = \ldots = a_i^{n,i} = 1$, which corresponds to $P_i^{(n)}(1) = 1$.

As we can see from the above explicit expression of $P_i^{(n)}$, the determinant $d_i^{(n)}$ can be zero. This depends on the values assigned to $a_0^{n,i}, a_1^{n,i}, \ldots, a_i^{n,i}$, that is, on the normalization. When $P_i^{(n)}$ is singular, $d_i^{(n)}$ is zero. In this situation, we say that there is a *breakdown*. The aim of this work is to introduce new regular biorthogonal polynomials with some normalization and to use them in the computation of regular orthogonal polynomials in order to avoid breakdown problems.

Let $\{P_i^{\theta_n}\}_{n,i}$ be a family of monic polynomials such that, for all i, $P_i^{\theta_n}$ has degree i and

$$C^{(n)}(x^{\theta_n(j)} P_i^{\theta_n}) = 0, \qquad j = 0, 1, \ldots, i-1. \tag{2}$$

The family $\{P_i^{\theta_n}\}_{n,i}$ contains all the monic regular orthogonal polynomials with respect to $C^{(n)}$. The explicit expression of each polynomial $P_i^{\theta_n}$ is

$$P_i^{\theta_n}(x) = \begin{vmatrix} c_{\theta_n(0)+n} & c_{\theta_n(0)+n+1} & \cdots & c_{\theta_n(0)+n+i} \\ c_{\theta_n(1)+n} & c_{\theta_n(1)+n+1} & \cdots & c_{\theta_n(1)+n+i} \\ \vdots & \vdots & & \vdots \\ c_{\theta_n(i-1)+n} & c_{\theta_n(i-1)+n+1} & \cdots & c_{\theta_n(i-1)+n+i} \\ 1 & x & \cdots & x^i \end{vmatrix} / H_i^{\theta_n}.$$

This shows that $P_i^{\theta_n}$ is a regular orthogonal polynomial if and only if

$$\theta_n(\{0, 1, \ldots, i-1\}) = \{0, 1, \ldots, i-1\}.$$

In particular, when θ_n is the identity, we recover the explicit expressions of adjacent orthogonal polynomials which are studied, in the normal case, in [5]. When $P_i^{\theta_n}$ is not orthogonal with respect to $C^{(n)}$, it is, in fact, a biorthogonal polynomial, as defined in [2].

3. Recurrence relations. Assume that there exists a regular orthogonal polynomial $P_k^{\theta_n}$ such that

$$C^{(n)}(x^k P_k^{\theta_n}) = 0.$$

From the explicit expression of $P_k^{\theta_n}$, we get $C^{(n)}(x^{\theta_n(k)}P_k^{\theta_n}) = H_{k+1}^{\theta_n}/H_k^{\theta_n} \neq 0$. In the following theorem, we see how to compute the biorthogonal polynomials $P_{k+1}^{\theta_n}, P_{k+2}^{\theta_n}, \ldots, P_{\theta_n(k)}^{\theta_n}$ of the family $\{P_i^{\theta_n}\}_i$, for a fixed integer n.

Theorem 3.1. *For* $i \in \{k, \ldots, \theta_n(k) - 1\}$, *we have*

(i) $P_{i+1}^{\theta_n} = xP_i^{\theta_n} + \alpha_i P_k^{\theta_n}$ *with*

$$\alpha_i = -C^{(n)}(x^{\theta_n(k)+1}P_i^{\theta_n})/C^{(n)}(x^{\theta_n(k)}P_k^{\theta_n}),$$

(ii) $C^{(n)}(x^j P_{i+1}^{\theta_n}) = 0$ *for* $j = 0, \ldots, \theta_n(k)$ *and* $j = \theta_n(k) + k - (i+1)$,

(iii) $\theta_n(i+1) = \theta_n(k) + k - (i+1)$ *and*

$$C^{(n)}(x^{\theta_n(i+1)}P_{i+1}^{\theta_n}) = C^{(n)}(x^{\theta_n(k)}P_k^{\theta_n}) \neq 0.$$

Proof. The proof is by induction on i from $i = k$. It consists in proving that $xP_i^{\theta_n} + \alpha_i P_k^{\theta_n}$ satisfies the orthogonality condition (2) for $P_{i+1}^{\theta_n}$. ∎

This theorem shows that $P_{\theta(k)+1}^{\theta_n}$ is a regular orthogonal polynomial and that $P_k^{\theta_n}$ divides $P_i^{\theta_n}$ for $i = k, k+1, \ldots, \theta_n(k)$.

Theorem 3.2. *Let* $P_{k_0}^{\theta_n}$ *be the regular orthogonal polynomial of the highest degree preceding* $P_k^{\theta_n}$. *Then* $P_{\theta_n(k)+1}^{\theta_n}$ *can be computed from the recurrence relation*

$$P_{\theta_n(k)+1}^{\theta_n} = xP_{\theta_n(k)}^{\theta_n} + \sum_{i=k+1}^{\theta_n(k)} \alpha_i P_i^{\theta_n} + \alpha_k P_k^{\theta_n} + \alpha_{k-1} P_{k_0}^{\theta_n}$$

with

$$\alpha_{k-1} = -C^{(n)}(x^{\theta_n(k)}P_k^{\theta_n})/C^{(n)}(x^{\theta_n(k_0)}P_{k_0}^{\theta_n}) \neq 0,$$

$$\alpha_k = -(C^{(n)}(x^{\theta_n(k)+1}P_{\theta_n(k)}^{\theta_n}) + \alpha_{k-1}C^{(n)}(x^{\theta_n(k)}P_{k_0}^{\theta_n}))/C^{(n)}(x^{\theta_n(k)}P_k^{\theta_n}),$$

$$\alpha_i = C^{(n)}(x^{\theta_n(i)}P_{k_0}^{\theta_n})/C^{(n)}(x^{\theta_n(k_0)}P_{k_0}^{\theta_n}), \qquad i = k+1, \ldots, \theta(k).$$

Proof. Since $P_{k_0}^{\theta_n}$ is the regular orthogonal polynomial of the highest degree preceding $P_k^{\theta_n}$, we have $\theta_n(k_0) = k - 1$. For fixed n, the set $\{P_i^{\theta_n}\}_i$ is a basis of $\mathbb{C}[X]$, so we can write

$$P_{\theta_n(k)+1}^{\theta_n} = xP_{\theta_n(k)}^{\theta_n} + \sum_{i=0}^{\theta_n(k)} \alpha_i P_i^{\theta_n}. \tag{3}$$

Multiplying (3) by $x^{\theta_n(j)}$ and applying $C^{(n)}$ gives the expressions for α_i and shows that (3) is equivalent to

$$P_{\theta_n(k)+1}^{\theta_n} = xP_{\theta_n(k)}^{\theta_n} + \sum_{i=k+1}^{\theta_n(k)} \alpha_i P_i^{\theta_n} + \alpha_k P_k^{\theta_n} + \alpha_{k_0} P_{k_0}^{\theta_n}. \tag{4}$$ ∎

By Theorems 3.1 and 3.2, there exists a polynomial $W_{\theta_n(k)-k+1}(x)$ of degree $\theta_n(k)-k+1$ such that $P^{\theta_n}_{\theta(k)+1}(x) = W_{\theta_n(k)-k+1}(x)P^{\theta_n}_k(x)+\alpha_{k-1}P^{\theta_n}_{k_0}(x)$. It is sufficient to remark that P_k divides $P^{\theta_n}_i$ for $i = k, \ldots, \theta_n(k)$. Different proofs of this property were given by Draux [16], Gragg and Lindquist [19] and Gutknecht [21]. Notice that our proof is shorter and simpler than that of Gutknecht [21].

The polynomials $P^{\theta_n}_q$ can be displayed in an array called the *table* P. We suppose that this table P contains a square block of order $\theta_n(k) - k$ at its kth column. This can be illustrated by the scheme

$$\begin{array}{c|cc}
P^{\theta_n}_k & P^{\theta_{n-1}}_{k+1} & \cdots \\ \hline
P^{\theta_{n+1}}_k & P^{\theta_n}_{k+1} & \cdots \\
P^{\theta_{n+2}}_k & P^{\theta_{n+1}}_{k+1} & \cdots \\
\vdots & \vdots & \ddots
\end{array}$$

where $P^{\theta_n}_k$ is regular. From the preceding results, we obtain the two relations

$$\begin{cases} P^{\theta_{m+1}}_k = P^{\theta_m}_k - e^{\theta_m}_k P^{\theta_{m+1}}_{\theta_{m+1}(k-1)}, \\ e^{\theta_m}_k = C^{(m)}(x^k P^{\theta_m}_k)/C^{(m+1)}(x^{k-1}P^{\theta_{m+1}}_{\theta_{m+1}(k-1)}), \end{cases}$$

for $m = n, \ldots, n + \theta_n(k) - k$, and

$$\begin{cases} P^{\theta_{m-1}}_{i+1} = xP^{\theta_m}_i - q^{\theta_{m-1}}_{i+1} P^{\theta_{m-1}}_{\theta_{m-1}(i)}, \\ q^{\theta_{m-1}}_{i+1} = C^{(m)}(x^i P^{\theta_m}_i)/C^{(m-1)}(x^i P^{\theta_{m-1}}_{\theta_{m-1}(i)}), \end{cases}$$

for $i = k, \ldots, \theta_n(k)$, $m = n + k - i$. These relations yield some properties of blocks of the table P:

THEOREM 3.3 *For every $n \in \mathbb{Z}$, if the table P contains a block at its kth column as described above, then*

$$P^{\theta_{n+i}}_k = P^{\theta_n}_k, \qquad P^{\theta_{n-i}}_{k+i} = x^i P^{\theta_n}_k, \qquad i = 0, \ldots, \theta_n(k) - k,$$

with $\theta_{n-i}(k + i) = \theta_n(k)$ and $\theta_{n+i}(k) = \theta_n(k) - i$ for $i = 0, \ldots, \theta_n(k) - k$.

This was proved by Draux in [16]. Here, we only made the connection with the permutation θ_n, which simplifies the recurrence relations. We also note that a simple proof of this theorem can be deduced from (5) and (6). ■

The new biorthogonal polynomials defined above are displayed inside the blocks of the table P.

THEOREM 3.4. *For every $n \in \mathbb{Z}$, if the table P has a block at its kth column as described above, then for $i=k, \ldots, \theta_n(k)$ and $m=0, \ldots, \theta_n(k)-i$,* *we have*

$$P_i^{\theta_{n+m}} = P_i^{\theta_n}, \qquad P_{i+m}^{\theta_{n-m}} = x^m P_i^{\theta_n},$$
$$\theta_{n-m}(i+m) = \theta_n(i), \qquad \theta_{n+m}(i) = \theta_n(i) - m.$$

Proof. We use the properties of the permutation θ_n given in Theorems 3.3 and 3.1. Indeed, from Theorem 3.1, $\theta_{n-m}(i+m) = \theta_{n-m}(i+m-1)+1$, and from Theorem 3.3, $\theta_{n-m}(i+m-1)+1 = \theta_{n-m+1}(i+m-1)$. Thus, by applying Theorem 3.1 and then Theorem 3.3, m times, we deduce that $\theta_{n-m}(i+m) = \theta_n(i)$.

Theorem 3.3 shows that $\theta_{n+m}(i) = \theta_{n+m-1}(i) - 1$. By applying Theorem 3.3, m times, we get $\theta_{n+m}(i) = \theta_n(i) - m$.

These relations between the permutations θ_j show that $P_i^{\theta_n}$ and $x^m P_i^{\theta_n}$ have the properties of $P_i^{\theta_{n+m}}$ and $P_{i+m}^{\theta_{n-m}}$ respectively, so $P_i^{\theta_{n+m}} = P_i^{\theta_n}$ and $P_{i+m}^{\theta_{n-m}} = x^m P_i^{\theta_n}$. ∎

Theorem 3.4 is a generalization of Theorem 3.3.

By using the recurrence relations of Theorems 3.1 and 3.2, we can derive an algorithm for computing the regular orthogonal polynomials with respect to the functional $C^{(n)}$. Actually, this algorithm allows one to move along a diagonal of the table P. It makes use of the intermediate biorthogonal polynomials for computing the regular orthogonal ones. The procedure is called ALA (Avoiding Look-Ahead strategy).

3.1. *Implementation of ALA.* Define a symmetric bilinear form g_1 on $\mathbb{C}[X]$ by

$$g_1(\psi, \varphi) = C(\psi\varphi), \qquad \forall \psi, \varphi \in \mathbb{C}[X].$$

For simplicity, we write C and θ instead of $C^{(n)}$ and θ_n since n is fixed.

Definition 3.1. Let $D = \{p_0, p_1, \ldots\}$ and $Q = \{q_0, q_1, \ldots\}$ be two sets of polynomials. If $g_1(p_i, q_j) = 0$ for $i \neq j$, then we say that D and Q are g_1-*biorthogonal*.

We consider two bases $\{v_0, v_1, \ldots\}$ and $\{w_0, w_1, \ldots\}$ of $\mathbb{C}[X]$ such that, for every integer i, the polynomials v_i and w_i are of degree i. We assume that $(\mathbb{C}[X], g_1)$ is regular. A subspace $L \times L'$ of $\mathbb{C}[X] \times \mathbb{C}[X]$ is called *regular* if the right-orthogonal of L,

$$L^{\perp_{g_1}} = \{z \in \mathbb{C}[X] \mid \forall y \in L,\ g_1(y,z) = 0\},$$

does not contain any element of L', and the left-orthogonal of L',

$$L'^{g_1\perp} = \{y \in \mathbb{C}[X] \mid \forall z \in L',\ g_1(y,z) = 0\},$$

is such that $L \cap L'^{g_1\perp} = \{0\}$.

As $(\mathbb{C}[X], g_1)$ is regular, we can choose two permutations σ and θ of $\mathbb{N}$ such that, for every integer i, the subspace $V_i^\sigma \times W_i^\theta$ generated by $\{v_{\sigma(0)}, \ldots$

$\ldots, v_{\sigma(i)}\} \times \{w_{\theta(0)}, \ldots, w_{\theta(i)}\}$ is regular. This choice enables us to build two g_1-biorthogonal bases $D = \{p_0, p_1, \ldots\}$ and $Q = \{q_0, q_1, \ldots\}$ of monic polynomials such that, for every integer i, $p_i \in V_i^\sigma \backslash V_{i-1}^\sigma$ and $q_i \in W_i^\theta \backslash W_{i-1}^\theta$. For more details, see [2].

To each pair of bases $\{v_0, v_1, \ldots\}$ and $\{w_0, w_1, \ldots\}$, there corresponds another pair of bases which are g_1-biorthogonal. We are interested in the choice of $\{v_0, v_1, \ldots\}$ and $\{w_0, w_1, \ldots\}$ which yields all the regular orthogonal polynomials with respect to the functional C. This means that the corresponding g_1-biorthogonal bases $\{p_0 = P_0^\theta, p_1 = P_1^\theta, \ldots\}$ and $\{q_0 = Q_{\theta(0)}^\theta, q_1 = Q_{\theta(1)}^\theta, \ldots\}$ satisfy $Q_i^\theta = P_i^\theta = P_i$ for every monic regular orthogonal polynomial P_i of degree i.

We will introduce three interesting choices which give three different ways for implementing the ALA method. These choices will be called C1, C2 and C3.

We now give the recurrence relations connecting the polynomials of $\{P_0^\theta, P_1^\theta, \ldots\}$ and $\{Q_{\theta(0)}^\theta, Q_{\theta(1)}^\theta, \ldots\}$, in order to apply them to the Lanczos method. This is equivalent to substituting y for the variable x of the polynomials Q_i^θ, in order to have two biorthogonal bases with respect to the bilinear form g_2 defined on $\mathbb{C}[X] \times \mathbb{C}[Y]$ by $g_2(x^i, y^j) = C(x^{i+j})$ for $i, j \in \mathbb{N}$.

• C1 is obtained by taking for σ the identity permutation and by choosing recursively the polynomials of the bases $\{v_0, v_1, \ldots\}$ and $\{w_0, w_1, \ldots\}$ with $v_j = xP_{j-1}^\theta$ and $w_j = x^j$ for $j = 1, 2, \ldots$ This choice was already studied in Section 2 and before this subsection.

• C2 consists in setting

$$\begin{aligned} v_j &= xP_{j-1}^\theta, && j = 1, 2, \ldots, \\ w_j &= x^{j-k} Q_k^\theta, && j = k+1, \ldots, \theta(k)+1, \\ & && k = 0, \theta(0)+1, \theta(\theta(0)+1)+1, \ldots \end{aligned}$$

The degrees of the polynomials v_j and w_j are equal to their indices. The definitions of P_j^θ and Q_j^θ yield the recurrence relations

$$Q_j^\theta = x^{j-k} Q_k^\theta, \qquad j = k+1, \ldots, \theta(k), \tag{7}$$

$$\begin{cases} \alpha_{j-1} = C(xP_{j-1}^\theta Q_{\theta(k)}^\theta)/C(P_k^\theta Q_{\theta(k)}^\theta), \\ P_j^\theta = xP_{j-1}^\theta - \alpha_{j-1} P_k^\theta, \end{cases} \qquad j = k+1, \ldots, \theta(k), \tag{8}$$

$$\begin{cases} \alpha_{\theta(k)} = C(xP_{\theta(k)}^\theta Q_{\theta(k)}^\theta)/C(P_k^\theta Q_{\theta(k)}^\theta), \\ \beta_{\theta(k)} = C(P_{\theta(k)}^\theta Q_k^\theta)/C(P_{\theta(k-1)}^\theta Q_{k-1}^\theta), \\ P_{\theta(k)+1}^\theta = xP_{\theta(k)}^\theta - \alpha_{\theta(k)} P_k^\theta - \beta_{\theta(k)} P_{\theta(k-1)}^\theta, \\ Q_{\theta(k)+1}^\theta = xQ_{\theta(k)}^\theta - \displaystyle\sum_{i=k+1}^{\theta(k)} \alpha_{\theta(i)} Q_i^\theta - \alpha_{\theta(k)} Q_k^\theta - \beta_{\theta(k)} Q_{\theta(k-1)}^\theta. \end{cases} \tag{9}$$

For every i, if the polynomials Q_i^θ and P_i^θ are both orthogonal, then $Q_i^\theta = P_i^\theta$. Replacing Q_i^θ by P_i^θ if $Q_i^\theta = P_i^\theta$, these three equations lead to an implementation of the ALA method where only three vectors need to be stored.

The coefficients $\alpha_{\theta(i)}$ of the relation which gives $Q_{\theta(k)+1}^\theta$ can also be computed by using the polynomials of the set $\{P_{k-1}'^\theta, P_k'^\theta, \ldots, P_{\theta(k)}'^\theta, P_{\theta(k)+1}'^\theta\}$ which is g_1-biorthogonal to $\{xQ_{\theta(k)}^\theta, Q_{\theta(k)}^\theta, Q_{\theta(k)-1}^\theta, \ldots, Q_k^\theta, Q_{\theta(k-1)}^\theta\}$ with $P_{k-1}'^\theta = P_{k-1}^\theta$. The computation of the polynomials $P_i'^\theta$ is via the following relation which connects them to P_i^θ:

$$\text{(10)} \qquad \begin{cases} \lambda_i = C(P_i^\theta x Q_{\theta(k)}^\theta)/C(P_k^\theta Q_{\theta(k)}^\theta), \\ P_i'^\theta = P_i^\theta - \lambda_i P_{k-1}^\theta, \end{cases} \qquad i = k, k+1, \ldots, \theta(k)+1.$$

Thanks to these polynomials, the expression for $\alpha_{\theta(i)}$ is

$$\alpha_{\theta(i)} = -\beta_{\theta(k)} C(Q_{\theta(k-1)}^\theta P_{\theta(i)}'^\theta)/C(Q_i^\theta P_{\theta(i)}'^\theta).$$

If we only need to compute P_j^θ, then we can use the simpler relation

$$\text{(11)} \quad \begin{cases} \alpha_j = C(x^{\theta(k)-k+1} P_j^\theta P_k^\theta)/C(x^{\theta(k)-k} P_k^\theta P_k^\theta), \\ \beta_j = C(P_j^\theta P_k^\theta)/C(P_{\theta(k-1)}^\theta P_{k-1}^\theta), \\ P_{j+1}^\theta = x P_j^\theta - \alpha_j P_k^\theta - \beta_j P_{\theta(k-1)}^\theta, \end{cases} \qquad j = k, k+1, \ldots, \theta(k),$$

for $k = 0, \theta(0)+1, \theta(\theta(0)+1)+1, \ldots$ The initializations of this recurrence relation are $P_0^\theta = 1$ and $P_{-1}^\theta = 0$ with $\theta(-1) = -1$.

- C3 consists in taking

$$\begin{aligned} v_j &= x^{j-k} P_k^\theta, && j = k+1, k+2, \ldots, n_k, \\ v_{j+1} &= x P_j^\theta, && j = n_k, n_k+1, \ldots, \theta(k), \\ w_j &= x^{j-k} Q_k^\theta, && j = k+1, k+2, \ldots, n_k, \\ w_{j+1} &= x Q_j^\theta, && j = n_k, n_k+1, \ldots, \theta(k), \end{aligned}$$

for $k = 0, \theta(0)+1, \theta(\theta(0)+1)+1, \ldots$, with $n_k = \lfloor(\theta(k)+k+1)/2\rfloor$. The degrees of v_j and w_j are equal to their indices. For a complete study of this choice, see [2].

For C2, we deduce from (11) the following theorem which generalizes the classical recurrence relation for regular orthogonal polynomials.

Theorem 3.5. *Every regular orthogonal polynomial $P_{\theta(k)+1}^\theta$ satisfies a recurrence relation of the form*

$$P_{\theta(k)+1}^\theta = x P_{\theta(k)}^\theta - \alpha_{\theta(k)} P_k^\theta - \beta_{\theta(k)} P_{\theta(k-1)}^\theta,$$

where P_k^θ is the regular orthogonal polynomial of the highest degree preceding

$P^{\theta}_{\theta(k)+1}$. *The degrees of* $P^{\theta}_{\theta(k)+1}$, $P^{\theta}_{\theta(k)}$, P^{θ}_{k} *and* $P^{\theta}_{\theta(k-1)}$ *are equal to their lower indices.*

In the following, we are most interested in the application of C2 because of its particular characteristics which are detailed in [2].

4. Application to the Lanczos method. Let us begin by describing the Lanczos method following [13, 14].

4.1. *Description.* We want to find the solution of the linear system $Ax = b$, where $A \in \mathbb{C}^{n\times n}$ is supposed to be non-singular, $b \in \mathbb{C}^n$ and $x \in \mathbb{C}^n$.

Let x_0 and y_0 be arbitrary vectors in $\mathbb{C}^n$ and define two sequences $(x_k)_k$ and $(r_k)_k$ of vectors by

$$x_k - x_0 \in K_k(A, r_0), \tag{12}$$

$$r_k = b - Ax_k \perp K_k(A^*, y_0), \tag{13}$$

where $K_k(A,r) = \operatorname{span}(r, Ar, \ldots, A^{k-1}r)$ and A^* denotes the conjugate transpose of the matrix A.

The Lanczos method is completely defined by (12) and (13). It consists recursively in projecting the initial residual r_0 on the Krylov space $K_k(A, Ar_0)$, orthogonally to $K_k(A^*, y_0)$ with respect to the Hermitian product $\langle\cdot,\cdot\rangle$ of $\mathbb{C}^n$. Here $\langle\cdot,\cdot\rangle$ replaces the form g_1 introduced before. From (12), we can write

$$x_k - x_0 = -\alpha_1 r_0 - \alpha_2 Ar_0 - \ldots - \alpha_k A^{k-1} r_0. \tag{14}$$

Multiplying (14) by A and subtracting b, we obtain

$$r_k = r_0 + \alpha_1 Ar_0 + \ldots + \alpha_k A^k r_0.$$

(13) implies

$$\langle r_k, A^{*i} y_0\rangle = 0 \qquad \text{for } i = 0, \ldots, k-1. \tag{15}$$

If we consider the polynomial $P_k(\xi) = 1 + \alpha_1\xi + \ldots + \alpha_k\xi^k$, then $r_k = P_k(A)r_0$. Let us now define the linear functional C on $\mathbb{C}[X]$ by $C(\xi^i) = c_i = \langle A^i r_0, y_0\rangle$, $i = 0, 1, \ldots$, and the functional $C^{(1)}$ by $C^{(1)}(\xi^i) = C(\xi^{i+1})$, $i = 0, 1, \ldots$ The polynomial P_k satisfies

$$C(\xi^i P_k(\xi)) = 0 \qquad \text{for } i = 0, \ldots, k-1, \qquad P_k(0) = 1.$$

So, P_k is a formal orthogonal polynomial with respect to the linear functional C normalized by the condition $P_k(0) = 1$.

Let $P_k^{(1)}$ be the monic polynomial of degree k satisfying

$$C^{(1)}(\xi^i P_k^{(1)}(\xi)) = 0 \qquad \text{for } i = 0, \ldots, k-1.$$

$(P_k^{(1)})_k$ and $(P_k)_k$ are called *adjacent families* [29]. We can easily see that, for each $k \in \mathbb{N}^*$, P_k and $P_k^{(1)}$ exist and are unique if and only if the Hankel determinant

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

is different from zero. In order to define uniquely the two sequences $(P_k^\theta)_k$ and $(P_k^{\theta_1})_k$ with only one permutation θ, $(P_k^\theta)_k$ and $(P_k^{\theta_1})_k$ will be normalized by $P_k^\theta(0) = 1$ and $P_k^{\theta_1}$ monic of degree k.

Even if P_k^θ is not orthogonal, we set $r_k = P_k^\theta(A)r_0$. The polynomial P_k^θ satisfies

$$C(\xi^{\theta(i)} P_k^\theta(\xi)) = 0 \qquad \text{for } i = 0, \dots, k-1, \quad P_k^\theta(0) = 1.$$

Consequently, (15) becomes

$$\langle r_k, A^{*\theta(i)} y_0 \rangle = 0 \quad \text{for } i = 0, \dots, k-1. \tag{16}$$

(16) is equivalent to the linear system

$$(S) \qquad \begin{cases} \alpha_1 c_{\theta(0)+1} + \alpha_2 c_{\theta(0)+2} + \dots + \alpha_k c_{\theta(0)+k} = -c_{\theta(0)}, \\ \alpha_1 c_{\theta(1)+1} + \alpha_2 c_{\theta(1)+2} + \dots + \alpha_k c_{\theta(1)+k} = -c_{\theta(1)}, \\ \dots \\ \alpha_1 c_{\theta(k-1)+1} + \alpha_2 c_{\theta(k-1)+2} + \dots + \alpha_k c_{\theta(k-1)+k} = -c_{\theta(k-1)}. \end{cases}$$

According to the definition of θ, the determinant of (S) is $H_k^{\theta_1} \neq 0$. So, (S) has a unique solution.

A survey of the various algorithms for implementing the Lanczos method is given in [14]. Here, we only present the application of ALA to Lanczos/Orthodir which is described in [24, 31].

4.2. *Lanczos/Orthodir.* Several Lanczos/Orthodir type algorithms were given, for example, in [14]. In particular, we cite the algorithm known as Biodir [21].

According to C2, we apply ALA to Lanczos/Orthodir. This is also equivalent to applying ALA to Biodir.

In order to compute P_{k+1}, we use the formula

$$\begin{cases} P_{i+1}^\theta = P_i^\theta - \lambda_i \xi P_i^{\theta_1}, \\ \lambda_i = C(P_k^\theta Q_{\theta(i)}^{\theta_1}) / C(\xi P_k^{\theta_1} Q_{\theta(k)}^{\theta_1}), \end{cases} \qquad i = k, k+1, \dots, \theta(k). \tag{17}$$

Its proof is by induction from $i = k$ to $i = \theta(k)$, it consists in proving that $P_i^\theta - \lambda_i \xi P_i^{\theta_1}$ satisfies the orthogonality condition (2) for P_{i+1}^θ. This formula requires the knowledge of the polynomials $P_i^{\theta_1}$, $Q_i^{\theta_1}$. These polynomials are obtained from (7)–(9) if we substitute $C^{(1)}$ for C and θ_1 for θ. Therefore, to apply ALA to Lanczos/Orthodir according to C2, we use the formulas (7)–(9) and (17).

Now, we are able to give an algorithm which allows avoiding the look-ahead strategy in Biodir. This algorithm consists of three steps:

• initialization,

• determination of the next existing regular orthogonal polynomial, which is equivalent to determining $\sigma(k)$ at the iteration k,

• computation of the iterates x_{k+1}, z_{k+1} and the residual vector r_{k+1} at the iteration k.

Set $z_k = P_k^{\theta_1}(A)r_0$ and $y_k = Q_k^{\theta_1}(A^*)y_0$ for $k = 0, 1, \ldots$

ALGORITHM 1

• STEP 1 (Initialization): Choose x_0 and y_0 arbitrary in $\mathbb{C}^n$, set $r_0 = b - Ax_0$, $z_0 = r_0$, $z_{-1} = y_{-1} = (0, 0, \ldots, 0)^t$, $h_{-1} = 1$, $\theta(-1) = -1$ and $k = 0$.

• STEP 2 (the determination of $\sigma(k)$):

1 $i = 0$

2 $e_i = \langle y_{k+i}, r_k \rangle$

$y_{k+i+1} = A^* y_{k+i}$

$h_{k+i} = \langle y_{k+i+1}, z_k \rangle$

if $|h_{k+i}| < tol$ for some tolerance tol, then

$i = i + 1$, go to 2

end (if)

$\theta(k) = k + i$.

• STEP 3:

$b_k = h_{\theta(k)}/h_{k-1}$

for $i = k, \ldots, \theta(k)$

$\lambda_i = e_{\theta(k)-i}/h_{\theta(k)}$

$x_{i+1} = x_i + \lambda_i z_i$

$r_{i+1} = r_i - \lambda_i A z_i$

$\beta_i = \langle y_{\theta(k)+1}, A z_i \rangle / h_{\theta(k)}$

$z_{i+1} = A z_i - \beta_i z_k$

$y_{\theta(k)+1} \leftarrow y_{\theta(k)+1} - \beta_i y_{\theta(i)}$

end (for)

$z_{\theta(k)+1} \leftarrow z_{\theta(k)+1} - b_k z_{\theta(k-1)}$

$y_{\theta(k)+1} \leftarrow y_{\theta(k)+1} - b_k y_{\theta(k-1)}$

$k = \theta(k) + 1$

go to 1

end.

It is important to notice that, for each iteration of this algorithm, we have a product of A and A^* by a vector and three inner products. The coding of this algorithm needs the storage of $9+m$ vectors, where $m = \max_k(\theta(k) - k + 1) < n$.

4.3. *Numerical results.* First, let us mention that the computations were performed on a computer working with 16 decimal digits in double precision and our tests were run using FORTRAN 77.

Let $\|r_k\|$ be the residual norm obtained, at iteration k, by Algorithm 1. The algorithm is stopped at the kth iteration if $\|r_k\| < eps$, where eps is a given tolerance.

EXAMPLE 1. Consider the example of [12]:

$$\begin{pmatrix} 0 & 0 & 0 & \dots & 0 & -1 \\ 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \\ \vdots \\ n \end{pmatrix} = \begin{pmatrix} -n \\ 1 \\ 2 \\ \vdots \\ n-1 \end{pmatrix}.$$

We take $n = 1000$ and choose $y_0 = (1, 0, 0, \dots, 0, 0, 1)^t$, $x_0 = (0, 0, \dots, 0)^t$. For $tol = 10^{-1}, 10^{-2}, \dots, 10^{-16}$, $eps = 10^{-12}$, we get

$$\theta(0) = 0, \qquad \theta(k) = 999 - k \quad \text{ for } k = 1, \dots, 998, \qquad \theta(999) = 999.$$

There is stagnation from $k = 1$ until iteration $k = 998$. At the end of this stagnation, we obtain $\|r_{999}\| = 1.58 \cdot 10^4$ and $\|r_{1000}\| = 9.55 \cdot 10^{-6}$.

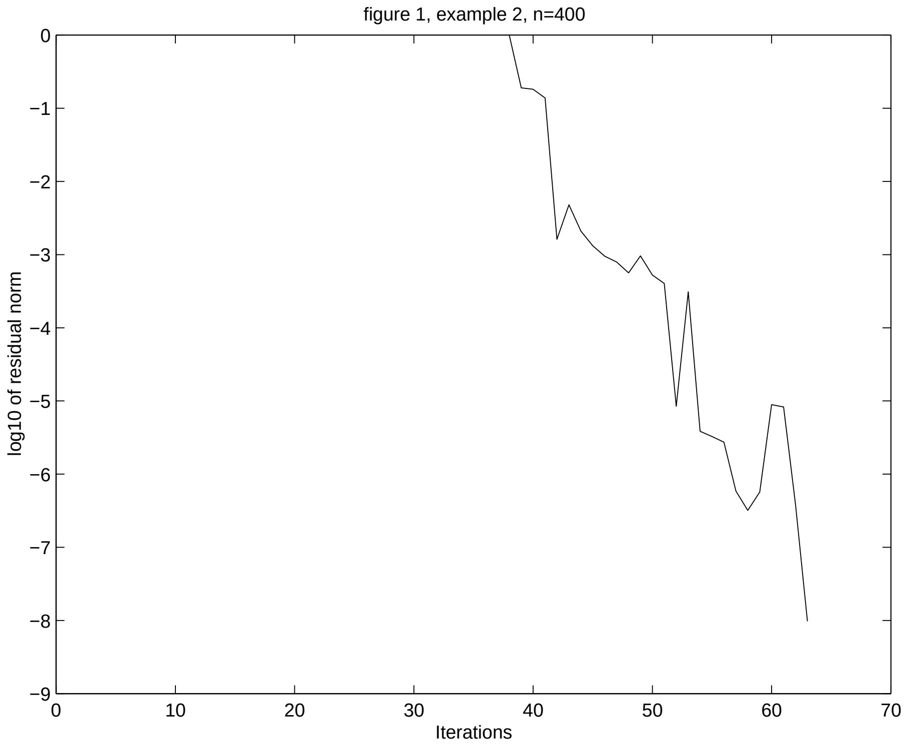
EXAMPLE 2. We consider a matrix obtained from discretization of the elliptic partial differential equation

$$Lu = f \qquad \text{on } [0,1] \times [0,1],$$

where

$$Lu = -\Delta u + s\frac{\partial u}{\partial x},$$

with Dirichlet boundary conditions $u = 0$, using a five-point centered finite difference scheme on a uniform 20×20 grid with mesh size $h = 1/21$. This yields a sparse non-symmetric matrix of order $n = 400$ with 1920 non-zero elements. We choose $s = 10^4$. By applying Algorithm 1 to this matrix with $tol = 10^{-1}, 10^{-2}, \dots, 10^{-16}$, $eps = 10^{-8}$, $y_0 = (0, 0, \dots, 0, 0, 1)^t$, $x_0 = (0, 0, \dots, 0)^t$, $b = (1, 0, 0, \dots, 0)^t$, we get



As for the first example, there is stagnation at the beginning. Afterwards, we obtain a good convergence to the exact solution. We also remark that the convergence curve presents some peaks. It is well known that these peaks are characteristic of Lanczos type methods.

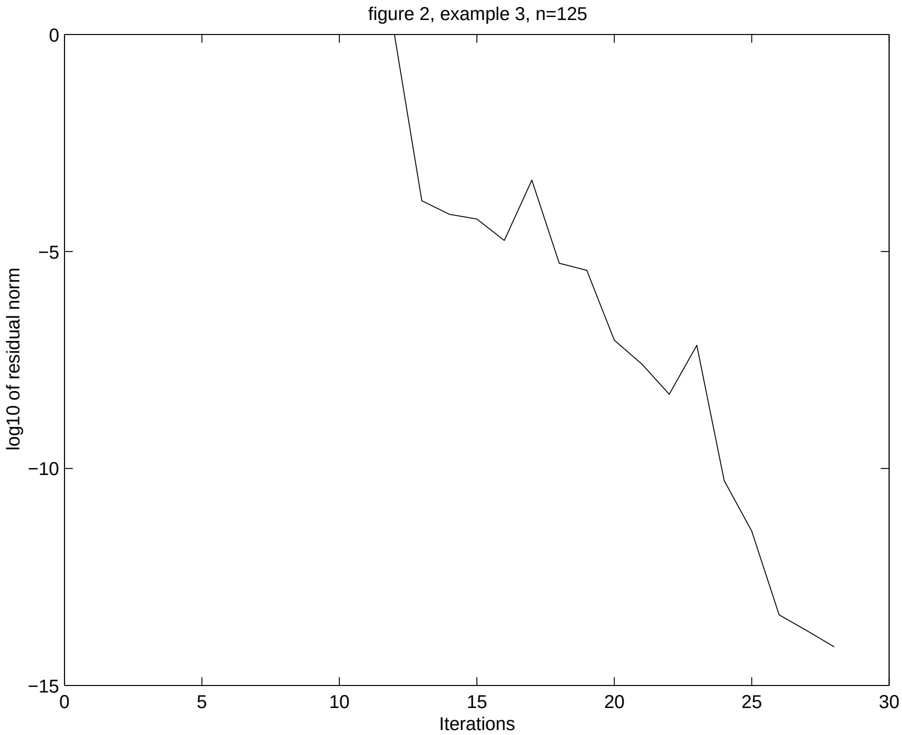
EXAMPLE 3. We consider a matrix arising from discretization of the 3-dimensional partial differential equation

$$Lu = f \qquad \text{on } [0,1] \times [0,1] \times [0,1],$$

where

$$Lu = -\Delta u + x\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y} + z\frac{\partial u}{\partial z} - u,$$

with Dirichlet boundary conditions $u = 0$. The operator was discretized using a seven-point centered finite difference scheme on a uniform $5 \times 5 \times 5$ grid with mesh size h equal to $1/6$. This yields a sparse non-symmetric matrix of order $n = 125$, with 725 non-zero elements. By using Algorithm 1 with $tol = 10^{-1}, 10^{-2}, \ldots, 10^{-16}$, $eps = 10^{-14}$, $y_0 = (0, 0, \ldots, 0, 0, 1)^t$, $x_0 = (0, 0, \ldots, 0)^t$, $b = (1, 0, 0, \ldots, 0)^t$, we obtain the following convergence curve:



For the values of the permutation θ, we get

$$\theta(k) = \begin{cases} 12 - k & \text{for } k = 0, 1, \dots, 12, \\ k & \text{for } k = 13, 14, \dots \end{cases}$$

At the beginning, we have stagnation from $k = 0$ until $k = 12$. After this stagnation, the residual norm converges quickly to zero. At iteration $k = 28$, we obtain $\|r_{28}\| = 7.52 \cdot 10^{-15}$.

Let us indicate that we have compared our estimation of the residual norm given by Algorithm 1 with the actual one. This comparison shows that both our estimation and the actual residual norm coincide.

4.4. *Application to the non-hermitian Lanczos process.* Define the symmetric bilinear form g_1 by $g_1(u, w) = w^t u$ for all $u, w \in \mathbb{C}^n$. According to C2, we get the following process.

Process 1. Choose $v_1, v_2 \in \mathbb{C}^n$ and set $\lambda_1 p_1 = v_1$, $\mu_1 q_1 = v_2$, $p_0 = 0$, $k = 1$ (λ_1 and μ_1 are chosen such that $\|p_1\| = \|q_1\| = 1$).

Compute

1 $i = 0$

2 $d_k = g_1(p_k, q_{k+i})$

if $|d_k| < tol$ (for some tolerance tol), then
  $i = i + 1$
  $\mu_{k+i} q_{k+i} = A^* q_{k+i-1}$ (μ_{k+i} is chosen such that $\|q_{k+i}\| = 1$)
  go to 2
end (if)
$\theta(k+j) = k + i - j, \;\; j = 0, 1, \ldots, i$
$q_{\theta(k)+1} = A^* q_{\theta(k)}$
for $j = k, k+1, \ldots, \theta(k)$:
  $\alpha_j = g_1(Ap_j, q_{\theta(k)}) / g_1(p_k, q_{\theta(k)})$
  $p_{j+1} = Ap_j - \alpha_j p_k$
  $\beta_j = g_1(q_{\theta(k)+1}, p_j) / g_1(q_{\theta(j)}, p_j)$
  $q_{\theta(k)+1} \leftarrow q_{\theta(k)+1} - \beta_j q_{\theta(j)}$
  if $j = \theta(k)$, then
    $\alpha'_j = g_1(Ap_j, q_{k-1}) / g_1(p_{\theta(k-1)}, q_{k-1})$
    $p_{j+1} \leftarrow p_{j+1} - \alpha'_j p_{\theta(k-1)}$
    $\beta'_j = g_1(q_{\theta(k)+1}, p_{k-1}) / g_1(q_{\theta(k-1)}, p_{k-1})$
    $\mu_{\theta(k)+1} q_{\theta(k)+1} \leftarrow q_{\theta(k)+1} - \beta'_j q_{\theta(k-1)}$
    ($\mu_{\theta(k)+1}$ is chosen such that $\|q_{\theta(k)+1}\| = 1$)
  end (if)
  $\lambda_{j+1} p_{j+1} \leftarrow p_{j+1}$ (λ_{j+1} is chosen such that $\|p_{j+1}\| = 1$)
end (for)
$k = \theta(k) + 1$, go to 1
end.

For solving a linear system, we use a process which allows us to triangularize, tridiagonalize or transform the matrix of the system to another one for which we have to find its inverse, as for example the Hessenberg matrix. Here, for each iteration k of Process 1, we get the following factorization:

$$A(p_k \; p_{k+1} \; \ldots \; p_{\theta(k)}) = (p_{\theta(k-1)} \; p_k \; p_{k+1} \; \ldots \; p_{\theta(k)} \; p_{\theta(k)+1}) \begin{pmatrix} d'^t_k \\ \widetilde{H}'_k \end{pmatrix}$$

where $d'^t_k = \alpha'_{\theta(k)}(0, 0, \ldots, 0, 1) \in \mathbb{C}^{\theta(k)-k+1}$, and the matrix $\widetilde{H}'_k$ with $\theta(k) - k + 2$ rows and $\theta(k) - k + 1$ columns is

$$\begin{pmatrix} \alpha_k & \alpha_{k+1} & \cdots & \alpha_{\theta(k)} \\ \lambda_{k+1} & & & \\ & \lambda_{k+2} & & \\ & & \ddots & \\ & & & \lambda_{\theta(k)+1} \end{pmatrix}.$$

Let us discuss the stopping criterion for this process. We consider two Krylov subspaces $W_2 = K_n(A, v_1) = \operatorname{span}(v_1, Av_1, A^2 v_1 \ldots)$ and $W_3 = K_n(A^*, v_2) = \operatorname{span}(v_2, A^* v_2, A^{*2} v_2, \ldots)$. There are two cases to consider:

• The first one corresponds to not having a breakdown at iteration k if $k \leq \min\{l, l'\}$ with $l = \dim W_2$ and $l' = \dim W_3$. This means that the subspace $(W_2 \times W_3, g_1)$ is regular.

• The second case is the situation where there is a serious incurable breakdown. It corresponds to a breakdown occurring at iteration k with $k \leq \min\{l, l'\}$ and it means that $(W_2 \times W_3, g_1)$ is not regular. Consequently, Process 1 cannot be used and the solution is to make another choice of the vectors v_1 and v_2 in $\mathbb{C}^n$.

Remark 4.1. This process needs the storage of $m + 5$ vectors of $\mathbb{C}^n$, where $m = \max_k\{\theta(k) - k + 1\}$. $m + 5$ is smaller than the number $2m + 4$ of vectors used in look-ahead strategies. In the regular case, the classical Lanczos process only needs 6 vectors. This number coincides with $m + 5$, since in the regular case, $\theta(k) = k$, which implies that $m = 1$ for all k.

We note that the factorization of Process 1 has also been used by Ziegler in [32, 33], where he talks about a special look-ahead strategy.

Remark 4.2. We have shown how to apply C2 to the Lanczos method. We can do the same for the CGM-type (Conjugate Gradient Multiplied) methods which have been simultaneously introduced by Brezinski [7] and Gutknecht [20], and which are also known under the name of "product-type methods". The CGM class contains CGS (Conjugate Gradient Squared) due to Sonneveld [27] and Bi-CGSTAB due to Van Der Vorst [28].

5. Application to Padé approximation.

Orthogonal polynomials and their associates implicitly come up in the computation of Padé approximants. Blocks of a non-normal Padé table are due to the non-existence and singularity of some orthogonal polynomials. In this section, we give relations between orthogonal, reciprocal, associated and intermediate polynomials introduced in [1], and we show how to apply them to the recursive computation of Padé approximants.

Let f be a formal power series $f(t) = c_0 + c_1t^1 + c_2t^2 + \ldots$ with $c_i \in \mathbb{C}$ for $i \in \mathbb{N}$. We look for a rational fraction

$$R(t) = \frac{Q(t)}{P(t)} = \frac{a_0 + a_1t + \ldots + a_pt^p}{b_0 + b_1t + \ldots + b_qt^q}$$

whose power series expansion in ascending powers of t agrees with f as far as possible, which means that $f(t) - R(t) = \mathcal{O}(t^{p+q+1})$ $(t \to 0)$. Such a rational fraction is called a *Padé approximant* of f and it is denoted by $[p/q]_f(t)$. Usually these approximants are displayed in a two-dimensional array called the *Padé table*. Identical Padé approximants can only occur in square blocks in the Padé table. If there is no block, we say that the Padé table is *normal*. Otherwise, it is called *non-normal*.

For every $n \in \mathbb{Z}$, define the linear functional $C^{(n)}$ on the space of complex polynomials by $C^{(n)}(x^i) = c_{n+i}$ with the convention that $c_i = 0$ for $i < 0$. $C^{(n)}$ is associated with the formal power series

$$f_n(t) = c_n + c_{n+1}t + c_{n+2}t^2 + \ldots$$

5.1. *The associated polynomials.* For every $P_q^{\theta_n}$, we consider the associated polynomial

$$Q_q^{\theta_n}(t) = C^{(n)}\left(\frac{P_q^{\theta_n}(x) - P_q^{\theta_n}(t)}{x - t}\right)$$

where $C^{(n)}$ acts on x.

LEMMA 5.1. *If $Q_k^{\theta_n}$ is associated with the polynomial $P_k^{\theta_n}$ of degree k, then*

$$Q_k^{\theta_n}(t) = \sum_{i=0}^{m} t^i C^{(n-i-1)}(P_k^{\theta_n}(x))$$

where $C^{(n-i-1)}$ acts on x and $m = n + k - 1 - \theta_n(0)$. $Q_k^{\theta_n}(t)$ has degree m if $m \geq 0$, otherwise $Q_k^{\theta_n}(t) = 0$.

Proof. $Q_k^{\theta_n}(t)$ is equal to $C^{(n)}[(P_k^{\theta_n}(x) - P_k^{\theta_n}(t))/(x - t)]$. By using the equality

$$1/(x - t) = x^{-1}\sum_{i=0}^{\infty}(x^{-1}t)^i,$$

we prove that

$$Q_k^{\theta_n}(t) = C^{(n)}\Big([P_k^{\theta_n}(x) - P_k^{\theta_n}(t)]x^{-1}\sum_{i=0}^{n+k-1}(x^{-1}t)^i\Big).$$

Finally, since $c_i = 0$ for $i < \theta(0)$, we obtain the result of the lemma. ■

5.2. *The reciprocal orthogonal polynomials.* We consider the reciprocal series g of $t^{-\theta(0)}f$ defined by $t^{-\theta(0)}f(t)g(t) = 1$. We set $g(t) = \sum_{i=0}^{\infty} d_i t^i$ and we define a functional $D^{(n)}$ on $\mathbb{C}[X]$ by $D^{(n)}(x^i) = d_{n+i}$ for $i \in \mathbb{N}$. $D^{(n)}$ is called the *reciprocal functional* of $C^{(n)}$. By convention, we set $d_i = c_i = 0$ if $i < 0$. Let η_n be the permutation associated with the functional $D^{(n)}$; it is called the *reciprocal permutation* of θ_n. We remark that the definition of $D^{(0)} = D$ implies $\eta(0) = \eta_0(0) = 0$. We will find later a relation which gives us the permutation η_n from θ_n. The complex numbers d_i are obtained from the equations

$$c_{\theta(0)}d_0 = 1, \quad c_{\theta(0)}d_j + c_{\theta(0)+1}d_{j-1} + \ldots + c_{\theta(0)+j}d_0 = 0 \quad \text{for } j = 1, 2, \ldots$$

An orthogonal polynomial with respect to $D^{(n)}$ is called *reciprocal*. We denote by $\{R_i^{\eta_n}\}_i$ the family of all these reciprocal orthogonal polynomials. They are useful for the recursive computation of numerators of Padé approximants. In the following theorem, we study the connection between the polynomials of the two families $\{P_i^{\theta_n}\}_{i,n}$ and $\{R_i^{\eta_n}\}_{i,n}$.

THEOREM 5.1. *If one of the polynomials* $P_k^{\theta_{\theta(0)+n+1}}$ *and* $R_{n+k}^{\eta_{-n+1}}$ *is regular and orthogonal, then so is the other. The same holds for* $P_{n+k}^{\theta_{\theta(0)-n+1}}$ *and* $R_k^{\eta_{n+1}}$. *If* $P_k^{\theta_{\theta(0)+n+1}}$ *and* $P_{n+k}^{\theta_{\theta(0)-n+1}}$ *are regular and orthogonal, then*

$$S_{n+k}^{\eta_{-n+1}} = d_0 P_k^{\theta_{\theta(0)+n+1}}, \quad Q_{n+k}^{\theta_{\theta(0)-n+1}} = c_{\theta(0)} R_k^{\eta_{n+1}}, \qquad n = 1, 2, \ldots,$$

$$\begin{cases} c_{\theta(0)} R_{n+k}^{\eta_{-n+1}} = P_k^{\theta_{\theta(0)+n+1}} \displaystyle\sum_{i=0}^{n} c_{\theta(0)+i} x^{n-i} + Q_k^{\theta_{\theta(0)+n+1}}, \\ d_0 P_{n+k}^{\theta_{\theta(0)-n+1}} = R_k^{\eta_{n+1}} \displaystyle\sum_{i=0}^{n} d_i x^{n-i} + S_k^{\eta_{n+1}}, \end{cases} \qquad n = 0, 1, \ldots$$

Proof. It is sufficient to remark that $f_{\theta(0)}$ is the reciprocal series of g (this means that $C^{(\theta(0))}$ is the reciprocal functional of D) and then use the results of [5, 16]. When $\theta(0) = 0$, the proof given in [5, 4] of the equalities of this theorem is long. It consists in transforming the determinants of the explicit expressions of the orthogonal polynomials. A simple proof is obtained by using only Lemma 5.1 (see the proof of Theorem 5.2). ■

From this theorem, it is clear that, for a fixed integer n, $R_{n+k}^{\eta_{-n+1}}$, $S_{n+k}^{\eta_{-n+1}}$, $P_k^{\theta_{\theta(0)+n+1}}$ and $Q_k^{\theta_{\theta(0)+n+1}}$ satisfy the same recurrence relations with different initializations. The same holds for $P_{n+k}^{\theta_{\theta(0)-n+1}}$, $Q_{n+k}^{\theta_{\theta(0)-n+1}}$, $R_k^{\eta_{n+1}}$ and $S_k^{\eta_{n+1}}$. If we set, for every $n, k \in \mathbb{N}$, $N_k^{\eta_{n+2}} = c_{\theta(0)} R_k^{\eta_{-n}}$ and $N_k^{\eta_{-n+1}} = c_{\theta(0)} R_k^{\eta_{n+1}}$, then the Padé approximant $[p/q]_f$ can be written as $[p/q]_f = \widetilde{N}_p^{\eta_{p-q+1}} / \widetilde{P}_q^{\theta_{\theta(0)+p-q+1}}$ whenever $P_q^{\theta_{\theta(0)+p-q+1}}$ is regular (see [5]).

We deduce from the preceding results that whether or not there are blocks in the Padé table, the numerator of each Padé approximant can be computed recursively by using the recurrence relations satisfied by the denominators.

COROLLARY 5.1. *The permutations* η_n *are connected to* θ_n *by the following relations*:

$$\begin{aligned} \eta_{-n+1}(i) &= \theta_{\theta(0)+n+1}(i-n) + n, \\ \theta_{\theta(0)-n+1}(i) &= \eta_{n+1}(i-n) + n \quad \textit{for } i \geq n,\ n \geq 1, \\ \theta_{\theta(0)-n+1}(i) &= \eta_{-n+1}(i) = n - 1 - i \quad \textit{for } i = 0, 1, \ldots, n-1. \end{aligned}$$

Proof. The knowledge of the degrees of all the regular orthogonal polynomials implies that of η_n and θ_n, see Theorems 3.1 and 3.2. So, from the definition of the permutations θ_n, η_n and by using Theorem 5.1, we get the assertion. ■

The quantities $Q_{n+k}^{\theta_{\theta(0)-n+1}}$ and $P_k^{\theta_{\theta(0)+n+1}}\sum_{i=0}^n c_{\theta(0)+i}x^{n-i} + Q_k^{\theta_{\theta(0)+n+1}}$ intervene in the recursive computation of the numerators of the Padé approximants. These quantities do not satisfy the equalities of Theorem 5.1 when $P_k^{\theta_{\theta(0)+n+1}}$ and $P_{n+k}^{\theta_{\theta(0)-n+1}}$ are not orthogonal. For this reason, we give some properties of them below. For every $n \in \mathbb{Z}$ and $k \in \mathbb{N}$, we consider the monic polynomials $R_k'^{\eta_n}$ defined by

$$D^{(n)}(R_k'^{\eta_n}t^{\eta_n(j)}) + \alpha_{n,k}d_{\eta_n(j)-\eta_n(k)} = 0, \qquad j = 0,\ldots,k-1, \tag{18}$$

where $\alpha_{n,k}$ is a constant such that the solution $R_k'^{\eta_n}$ of (18) is monic. The role of these polynomials is to replace the polynomials $R_k^{\eta_n}$ in the equalities of Theorem 5.1. By substituting $R_k'^{\eta_n}$ for $R_k^{\eta_n}$, the results of Theorem 5.1 are true even if $P_k^{\theta_{\theta(0)+n+1}}$ and $P_{n+k}^{\theta_{\theta(0)-n+1}}$ are not orthogonal. Clearly, the family $\{R_k'^{\eta_n}\}_{n,k}$ is built in such a way that it contains all the regular orthogonal polynomials with respect to the functional $D^{(n)}$. From the definition of $R_k'^{\eta_n}$, we can easily see that the condition for their existence and unicity is the same as for the polynomials $R_k^{\eta_n}$. Therefore, for every k and n, the polynomial $R_k'^{\eta_n}$ exists, is unique and has degree k.

THEOREM 5.2. *We have*

$$Q_{n+k}^{\theta_{\theta(0)-n+1}} = c_{\theta(0)}R_k'^{\eta_{n+1}}, \qquad S_{n+k}'^{\eta_{-n+1}} = d_0P_k^{\theta_{\theta(0)+n+1}}, \qquad n = 1,2,\ldots,$$

$$\begin{cases} c_{\theta(0)}R_{n+k}'^{\eta_{-n+1}} = P_k^{\theta_{\theta(0)+n+1}}\displaystyle\sum_{i=0}^n c_{\theta(0)+i}x^{n-i} + Q_k^{\theta_{\theta(0)+n+1}}, \\ d_0P_{n+k}^{\theta_{\theta(0)-n+1}} = R_k'^{\eta_{n+1}}\displaystyle\sum_{i=0}^n d_ix^{n-i} + S_k'^{\eta_{n+1}}, \end{cases} \qquad n = 0,1,\ldots$$

P r o o f. We want to prove $Q_{n+k}^{\theta_{\theta(0)-n+1}} = c_{\theta(0)}R_k'^{\eta_{n+1}}$. First assume that $\theta(0) = 0$. In this case, thanks to Lemma 5.1, we have, for $j = 0,1,\ldots,k-1$,

$$\begin{aligned} D^{(n+1)}[Q_{n+k}^{\theta_{-n+1}}(t)t^{\eta_{n+1}(j)}] &= D^{(n+1)}\Big[\sum_{i=0}^k t^{i+\eta_{n+1}(j)}C^{(-n-i)}(P_{n+k}^{\theta_{-n+1}}(x))\Big] \\ &= \sum_{l=0}^{n+k} a_l \sum_{i=0}^k d_{i+\eta_{n+1}(j)+n+1}c_{-n-i+l} \end{aligned}$$

where $D^{(n+1)}$ acts on t, $C^{(-n-i)}$ acts on x and $P_{n+k}^{\theta_{-n+1}}(x) = \sum_{l=0}^{n+k} a_lx^l$. Since $\theta(0)$ is zero, Corollary 5.1 implies $\theta_{-n+1}(j+n) = \eta_{n+1}(j)+n$, and we conclude that

$$D^{(n+1)}[Q_{n+k}^{\theta_{-n+1}}(t)t^{\eta_{n+1}(j)}] = \sum_{l=0}^{n+k} a_l \sum_{i=0}^{l-n} d_{i+\theta_{-n+1}(j+n)+1}c_{-n-i+l}$$

$$
\begin{aligned}
&= -\sum_{l=0}^{n+k} a_l \sum_{i=0}^{\theta_{-n+1}(j+n)} d_{\theta_{-n+1}(j+n)-i} c_{-n+1+l-i} \\
&= -\sum_{i=0}^{\theta_{-n+1}(j+n)} d_{\theta_{-n+1}(j+n)-i} C^{(-n+1)}(x^i P_{n+k}^{\theta_{-n+1}}(x)) \\
&= -d_{\theta_{-n+1}(j+n)-\theta_{-n+1}(k+n)} C^{(-n+1)}(x^{\theta_{-n+1}(k+n)} P_{n+k}^{\theta_{-n+1}}(x)) \\
&= -d_{\eta_{n+1}(j)-\eta_{n+1}(k)} C^{(-n+1)}(x^{\theta_{-n+1}(k+n)} P_{n+k}^{\theta_{-n+1}}(x)).
\end{aligned}
$$

Consequently, we obtain $Q_{n+k}^{\theta_{-n+1}} = c_0 R_k^{\prime\eta_{n+1}}$.

If $\theta(0) \neq 0$, then $f_{\theta(0)}$ is the reciprocal series of g. So, we can use the same reasoning as above and conclude that $Q_{n+k}^{\theta_{\theta(0)-n+1}} = c_{\theta(0)} R_k^{\prime\eta_{n+1}}$. Similarly, we prove that $S_{n+k}^{\prime\eta_{-n+1}} = d_0 P_k^{\theta_{\theta(0)+n+1}}$.

The remaining two equalities are deduced from those just proved. Indeed, from the two preceding equalities, for fixed n, the polynomials $R_{n+k}^{\prime\eta_{-n+1}}$, $P_k^{\theta_{\theta(0)+n+1}}$ and $Q_k^{\theta_{\theta(0)+n+1}}$ satisfy the same recurrence relations. The same holds for $P_{n+k}^{\theta_{\theta(0)-n+1}}$, $R_k^{\prime\eta_{n+1}}$ and $S_k^{\prime\eta_{n+1}}$. So, the last two equalities are valid if they are initially. That is indeed the case since

$$
S_0^{\prime\eta_{n+1}} = Q_0^{\theta_{\theta(0)+n+1}} = 0, \qquad P_0^{\theta_{\theta(0)+n+1}} = R_0^{\prime\eta_{n+1}} = 1
$$

and

$$
R_n^{\prime\eta_{-n+1}} = \sum_{i=0}^{n} d_i x^{n-i}, \qquad P_n^{\theta_{\theta(0)-n+1}} = \sum_{i=0}^{n} c_{\theta(0)+i} x^{n-i}. \ \blacksquare
$$

This theorem generalizes the result of Brezinski [4, 5] concerning the normal case. Brezinski used properties of determinants, which makes the proof longer.

If we set, for every $n, k \in \mathbb{N}$, $N_k^{\prime\eta_{n+2}} = c_{\theta(0)} R_k^{\prime\eta_{-n}}$ and $N_k^{\prime\eta_{-n+1}} = c_{\theta(0)} R_k^{\prime\eta_{n+1}}$, then we conclude from this theorem that $\widetilde{N}_p^{\prime\eta_{p-q+1}} / \widetilde{P}_q^{\theta_{\theta(0)+p-q+1}}$ is a Padé approximant denoted by $[p/q]_f^{\theta}$. If $[p/q]_f^{\theta}$ is inside a block, then it is equal to the Padé approximant which is located either on the west side or the north side of this block and on the diagonal of $[p/q]_f^{\theta}$.

We can compute the coefficients of the numerator of a Padé approximant in two ways:

1. The first one uses the recurrence relations satisfied by the polynomials $P_q^{\theta_{\theta(0)+p-q+1}}$ which are located on the same diagonal of the table P, because, from Theorem 5.2, these recurrence relations can also be applied to the polynomials $N_p^{\prime\eta_{p-q+1}}$.

For C1, C2 and C3, the computation of the coefficients of the numerator of $[p/q]_f^\theta$ requires at most $2p-1$ multiplications and $2p-1$ additions. This supposes the knowledge of the two non-identical Padé approximants preceding $[p/q]_f^\theta$ and located on the same diagonal.

2. The second way uses the equations

$$\begin{aligned} a_0 &= c_0 b_0, \\ a_1 &= c_1 b_0 + c_0 b_1, \\ &\ \vdots \\ a_p &= c_p b_0 + c_{p-1} b_1 + \ldots + c_{p-q} b_q, \end{aligned} \tag{19}$$

which directly give the coefficients a_i of the numerator of

$$[p/q]_f^\theta(t) = \frac{a_0 + a_1 t + \ldots + a_p t^p}{b_0 + b_1 t + \ldots + b_q t^q}$$

from those of the denominator.

In that case, the algorithmic cost is about $(q+1)(q+2)/2 + (p-q)(q+1)$ multiplications, $q(q+1)/2 + (p-q)q$ additions if $p \geq q$, and $(p+1)(p+2)/2 + (q-p)(p+1)$ multiplications, $p(p+1)/2 + (q-p)p$ additions if $p \leq q$.

By comparing the two algorithmic costs, we see that it is better to use the second method if we want to compute only one approximant. But, when we need to compute more Padé approximants, the first method is better.

5.3. *Numerical results.* We use C2 to compute the coefficients of the denominator $P(t) = b_0 + b_1 t + \ldots + b_q t^q$ and numerator $Q(t) = a_0 + a_1 t + \ldots + a_p t^p$ of the Padé approximant $R(t) = [p/q]_f^\theta$ which is arbitrarily chosen. The resulting algorithm follows a particular diagonal of the Padé table. Given the degrees p and q and the moments c_i, $i = 0, 1, \ldots, p+q$, this algorithm gives the coefficients of the numerator and denominator of $[p/q]_f^\theta$. The algorithm follows the diagonal which contains $[p/q]_f^\theta$.

We mention that, in the following examples, the coefficients of P and Q are computed from the same recurrence relation with two different initializations.

Example 1. We take the power series expansion

$$f(t) = 1 + t^5 + t^9/2 + t^{13}/4 + t^{17}/8 + t^{21}/16 + \ldots$$

of the rational function $(1 - t^4/2 + t^5)/(1 - t^4/2)$ for $t \in\,]-\sqrt[4]{2}, \sqrt[4]{2}[$. For the threshold of the detection of blocks, we set $tol = 10^{-12}$. According to C2, the Padé table has several blocks. We obtain

$$[p/q]_f^\theta = [0/0]_f^\theta = 1 \qquad \text{for } p, q \in \{0, 1, 2, 3, 4\},$$

$$
\begin{aligned}
[p/q]_f^\theta &= [4i+1/0]_f^\theta \\
&= 1 + t^5 \sum_{j=0}^{i-1} t^{4j}/2^j \qquad \text{for } 4i+1 \geq p \leq 4i+4,\ q \in \{0,1,2,3\},\ i \geq 1,
\end{aligned}
$$

$$[p/q]_f^\theta = [0/5]_f^\theta = 1/(1-t^5) \qquad \text{for } p \in \{0,1,2,3\},\ q \in \{5,6,7,8\},$$

$$[p/q]_f^\theta = [5/4]_f^\theta = (1 - t^4/2 + t^5)/(1-t^4/2) \qquad \text{for } p \geq 5,\ q \geq 4.$$

The approximants $[0/0]_f^\theta$, $[5/0]_f^\theta$, $[0/5]_f^\theta$ and $[5/4]_f^\theta$ are at the corners of a block of order 4.

For a power series which converges to a rational function, as is the case here, $[p/q]_f^\theta = f$ when p and q are respectively greater than (or equal to) the degrees of the numerator and denominator of this function.

Let us now give, according to C2, the numerators and denominators which we obtain for two approximants located inside the same block.

$[p/q]_f^\theta = P/Q$	$[2/6]_f^\theta$	$[3/7]_f^\theta$
C2	$P = 1 + 2t$ $Q = 1 + 2t - t^5 - 2t^6$	$P = 1 + 2t + 4t^2$ $Q = 1 + 2t + 4t^2 - t^5 - 2t^6 - 4t^7$

We note that the numerator and denominator of $[2/6]_f^\theta$ are different from those of $[3/7]_f^\theta$, even if $[2/6]_f^\theta = [3/7]_f^\theta$.

Example 2. Consider the power series studied in [11],

$$
\begin{aligned}
f(t) = 1 + at + at^2 + \ldots + at^{m-1} + t^m + at^{m+1} + at^{m+2} + \ldots \\
+ at^{2m-1} + t^{2m} + at^{2m+1} + \ldots
\end{aligned}
$$

This is the expansion of $(1 + at + at^2 + \ldots + at^{m-1})/(1-t^m)$ for $t \in \,]-1, 1[$. By setting $a = 0.001$, $tol = 10^{-10}$, and $m = 7$, the application of C2 gives us the following values of the numerator and denominator of $[4/4]_f^\theta$ which is inside a block of order 4.

a_i, b_i	C2
a_0	0.1000000000000000D+01
a_1	0.9009000000000003D+00
a_2	0.8116200000000002D+00
a_3	0.7311870000000003D+00
a_4	−0.2621775600000001D+01
b_0	0.1000000000000000D+01
b_1	0.9000000000000002D+00
b_2	0.8100000000000001D+00
b_3	0.7290000000000001D+00
b_4	−0.2624400000000001D+01

EXAMPLE 3. Consider the power series $f(t) = \sum_{i=0}^{\infty} c_i t^i = t^3 - t^6/2 + t^9/3 - \dots$ which converges to $\ln(1+t^3)$ if $t \in\,]-1, 1]$.

We apply C2 to f to compute the elements of the main diagonal of the Padé table. The execution of the corresponding algorithm with $tol = 10^{-12}$, in order to obtain $[10/10]_f^{\theta}$, meets four blocks and shows that the approximant $[10/10]_f^{\theta}$ is inside the 4th block which is of order 2. $[9/9]_f^{\theta}$ is on the north side of this block. For $[10/10]_f^{\theta}$, we get

a_i, b_i	C2
a_3	0.1000000000000000D+01
a_6	0.9999999999999951D+00
a_9	0.1833333333333311D+00
b_0	0.1000000000000000D+01
b_3	0.1499999999999995D+01
b_6	0.5999999999999954D+00
b_9	0.4999999999999934D−01

The other coefficients are zero.

The exact value of ln(2) is 0.6931471805599453... Set now $t = 1$ and look for an approximation of the value of ln(2) by using the Padé approximants $[k+1/k]_f^{\theta}$ obtained by C2.

k	$S_{2k+1} = \sum_{i=0}^{2k+1} c_i$	C2
3	0.5000	0.66
6	0.5833	0.6923
9	0.6166	0.693121
12	0.6345	0.6931464
15	0.6456	0.693147158
18	0.6532	0.693147179
21	0.6587	0.693147180540
24	0.6628	0.69314718055935
27	0.6628	0.693147180559927
30	0.6687	0.6931471805599447
32	0.7163	0.6931471805599454

From these results, we remark that the sequence $([k+1/k]_f^{\theta})_k$ of Padé approximants converges faster than $(S_{2k+1})_k$.

Consider now the power series $h(t) = \sum_{i=0}^{\infty} c'_i t^i = t - t^2/2 + t^3/3 - \dots$ which converges to $\ln(1+t)$ if $t \in\,]-1, 1]$. We have $f(t) = h(t^3)$. This proves that $[p/q]_h^{\theta}(t^3)$ is the Padé approximant $[3p/3q]_f^{\theta}(t)$ of f for every $p, q \in \mathbb{N}$. The application of C2 to h with $t = 1$ shows that

$$[k+1/k]_h^{\theta}(1) = [3k+3/3k+2]_f^{\theta}(1) \qquad \text{for } k = 1, 2, \dots$$

For example, we get

$$[2/1]_h^\theta(1) = [6/5]_f^\theta(1) = 0.7,$$
$$[6/5]_h^\theta(1) = [18/17]_f^\theta(1) = 0.6931471849621315.$$

The application of ALA to f meets several blocks, but it is not the case for h. This allows us to say that ALA gives good results both in the normal and in the non-normal case.

6. Application to the ε-algorithm. The ε-algorithm due to Wynn [30] is defined by the relation

$$\varepsilon_{k+1}^{(n)} = \varepsilon_{k-1}^{(n+1)} + (\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)})^{-1}. \tag{20}$$

If $\varepsilon_0^{(n)} = \sum_{i=0}^n c_i t^i$ and $\varepsilon_{-1}^{(n)} = 0$, then we get the equality $\varepsilon_{2k}^{(n)} = [n+k/k]_f(t)$, which characterizes the ε-algorithm and which enables it to accelerate the convergence of certain sequences. The intermediate quantities $\varepsilon_{2k+1}^{(n)}$ have no special significance. The ε-algorithm suffers from a numerical instability. Indeed, an important cancellation error due to the difference $\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)}$ can affect the algorithm. This numerical instability can be avoided by using either the following progressive form:

$$\varepsilon_{k+1}^{(n+1)} = \varepsilon_{k+1}^{(n)} + (\varepsilon_{k+2}^{(n)} - \varepsilon_k^{(n+1)})^{-1},$$

or the particular rules due to Wynn and given by Brezinski in [6]. For more details about the numerical stability of extrapolation methods, see [9, 15].

In this section, we are concerned with the computation of the iterates $\varepsilon_{2j}^{(n)}$ with even indices. These iterates can be computed by the extension of the bordering method given by Piñar and Ramirez in [26], which is an extension of the method described in [3]. We can also use the extensions of the bordering method obtained by the application of the ALA method. Here, we will use ALA according to C2 for extending the bordering method, in order to give a simple algorithm for computing the quantities $\varepsilon_{2j}^{(n)}$.

For every $n \in \mathbb{Z}$ and $j \in \mathbb{N}$, we set $\varepsilon_{2j}^{(n)} = [n+j/j]_f^\theta(t)$. This implies

$$\varepsilon_{2j}^{(n-1)} = \sum_{i=0}^{n-1} c_i t^i + t^n [j-1/j]_{f_n}^\theta(t) \tag{21}$$

with $[j-1/j]_{f_n}^\theta(t) = \widetilde{Q}_j^{\theta_n}(t)/\widetilde{P}_j^{\theta_n}(t)$, $\widetilde{Q}_j^{\theta_n}(t) = t^{j-1} Q_j^{\theta_n}(t^{-1})$, $\widetilde{P}_j^{\theta_n}(t) = t^j P_j^{\theta_n}(t^{-1})$ and

$$f_n(t) = c_n + c_{n+1} t + c_{n+2} t^2 + \ldots$$

The polynomials of the family $\{P_j^{\theta_n}\}_j$ are obtained by C2. For every polynomial $P_j^{\theta_n}$, we impose the normalization condition $P_j^{\theta_n}(1) = 1$ instead of being monic of degree j. This family contains all the regular orthogonal polynomials $P_j = P_j^{\theta_n}$ with respect to the functional $C^{(n)}$ which satisfy $P_j(1) = 1$.

Consider now the family $\{P'_j\}_j$ of orthogonal polynomials with respect to the functional $C'^{(n)} = C^{(n+1)} - C^{(n)}$, requiring P'_j to be monic of degree j. A reasoning similar to the one used at the beginning of Section 4 shows that P'_j exists if and only if P_j does. So, by applying C2, we have a unique permutation θ_n and so the family $\{P_j'^{\theta_n}\}_j$.

For every integer j, we consider $Q_j^{\theta_n}$ and $Q_j'^{\theta_n}$ as the polynomials associated respectively with $P_j^{\theta_n}$ and $P_j'^{\theta_n}$, with respect to the functional $C^{(n)}$. This means that

$$Q_j^{\theta_n}(t) = C^{(n)}\left(\frac{P_j^{\theta_n}(t) - P_j^{\theta_n}(x)}{t-x}\right),$$

$$Q_j'^{\theta_n}(t) = C^{(n)}\left(\frac{P_j'^{\theta_n}(t) - P_j'^{\theta_n}(x)}{t-x}\right),$$

where $C^{(n)}$ acts on x. According to C2, we will compute the polynomials of the family $\{P_j'^{\theta_n}\}_j$ from the following relation which is equivalent to (11):

$$\tag{22} \begin{cases} \alpha_j = C'^{(n)}(x^{\theta_n(k)-k+1} P_j'^{\theta_n} P_k'^{\theta_n}) / C'^{(n)}(x^{\theta_n(k)} P_k'^{\theta_n}), \\ \beta_j = C'^{(n)}(x^k P_j'^{\theta_n}) / C'^{(n)}(x^{k-1} P_{\theta_n(k-1)}'^{\theta_n}), \\ P_{j+1}'^{\theta_n} = x P_j'^{\theta_n} - \alpha_j P_k'^{\theta_n} - \beta_j P_{\theta_n(k-1)}'^{\theta_n}, \end{cases}$$

for $j = k, k+1, \ldots, \theta_n(k)$ and $k = 0, \theta_n(0)+1, \theta_n(\theta_n(0)+1)+1, \ldots$, with initialization $P_0'^{\theta_n} = 1$, $P_{-1}'^{\theta_n} = 0$ and $\theta_n(-1) = -1$.

The polynomials of the family $\{P_j^{\theta_n}\}_j$ are computed from

$$\tag{23} \begin{cases} \lambda_j = C^{(n)}(P_k'^{\theta_n}) / C'^{(n)}(x^{\theta_n(k)} P_k'^{\theta_n}), \\ P_{j+1}^{\theta_n} = P_j^{\theta_n} - \lambda_j (x-1) P_j'^{\theta_n}, \end{cases} \qquad j = k, k+1, \ldots, \theta_n(k),$$

for $k = 0, \theta_n(0)+1, \theta_n(\theta_n(0)+1)+1, \ldots$ The proof of this relation is similar to that of (17). The recurrence relations (22) and (23) yield that the associated polynomials $Q_j'^{\theta_n}$ and $Q_j^{\theta_n}$ satisfy the two recurrence relationships

$$\tag{24} Q_{j+1}'^{\theta_n}(t) = t Q_j'^{\theta_n}(t) - \alpha_j Q_k'^{\theta_n}(t) - \beta_j Q_{\theta_n(k-1)}'^{\theta_n}(t) + C^{(n)}(P_j'^{\theta_n}(x))$$

and

$$\tag{25} Q_{j+1}^{\theta_n}(t) = Q_j^{\theta_n}(t) - \lambda_j [(t-1) Q_j'^{\theta_n}(t) + C^{(n)}(P_j'^{\theta_n}(x))]$$

for $j = k, k+1, \ldots, \theta_n(k)$ and $k = 0, \theta_n(0)+1, \theta_n(\theta_n(0)+1)+1, \ldots$, with initialization $Q_{-1}'^{\theta_n} = 0$, $Q_0^{\theta_n} = Q_0'^{\theta_n} = 0$ and $\theta_n(-1) = -1$. The coefficients α_j, β_j, λ_j and those of the relations (22) and (23) are the same.

The quantity $C^{(n)}(P_j'^{\theta_n}(x))$ can be computed recursively by using (22). Indeed, a simple application of $C^{(n)}$ to (22) gives us

$$C^{(n)}(P_{j+1}'^{\theta_n}) = C^{(n)}(xP_j'^{\theta_n}) - \alpha_j C^{(n)}(P_k'^{\theta_n}) - \beta_j C^{(n)}(P_{\theta_n(k-1)}'^{\theta_n}).$$

Now $C^{(n)}(xP_j'^{\theta_n}) = C^{(n)}((x-1)P_j'^{\theta_n}) + C^{(n)}(P_j'^{\theta_n})$ is equal to $C^{(n)}(P_j'^{\theta_n})$ if $j \neq \theta_n(0)$ and to $C^{(n)}(P_j'^{\theta_n}) + c_{n+\theta_n(0)+1} - c_{n+\theta_n(0)}$ if $j = \theta_n(0)$. From this, we can write the following recurrence relation:

$$a_{j+1} = a_j - \alpha_j a_k - \beta_j a_{\theta_n(k-1)} + \delta_{j\theta_n(0)}(c_{n+\theta_n(0)+1} - c_{n+\theta_n(0)}) \tag{26}$$

for the coefficients $a_i = C^{(n)}(P_i'^{\theta_n})$, where δ_{ij} is the Kronecker symbol.

In the expression of $\varepsilon_{2j}^{(n-1)}$, there is a division by the quantity $P_j^{\theta_n}(1)$. But $P_j^{\theta_n}(1) = 1$, so we avoid such a division and consequently, (21) implies $\varepsilon_{2j}^{(n-1)} = \sum_{i=0}^{n-1} c_i + Q_j^{\theta_n}(1)$.

Remark 6.1. Even if we take the simple case $t = 1$, the iterates $\varepsilon_{2j}^{(n-1)}$ can be computed to obtain an approximation of $[n+j-1/j]_f^{\theta}(t)$ for any fixed t not necessarily equal to 1. This is possible by substituting $c_i' = c_i t^i$ for c_i.

By using (25), we get

$$\varepsilon_{2j+2}^{(n-1)} = \varepsilon_{2j}^{(n-1)} - \lambda_j a_j \tag{27}$$

for $j = k, k+1, \ldots, \theta_n(k)$ and $k = 0, \theta_n(0)+1, \theta_n(\theta_n(0)+1)+1, \ldots$ To initialize this recurrence relation, we set $\varepsilon_0^{(n-1)} = \sum_{i=0}^{n-1} c_i$. From (23), the expression giving the coefficient λ_j does not depend on the polynomials $P_j'^{\theta_n}$. So, to compute the iterates $\varepsilon_{2j}^{(n-1)}$, we need (27), (26) and (22), to which we add (23), which gives λ_j. Now, we are ready to state the algorithm which computes the elements $\varepsilon_{2j}^{(n-1)}$ of even indices of the ε-array and which follows an arbitrary diagonal.

For every integer i, we set $P_i'^{\theta_n}(x) = \sum_{j=0}^{i} q_j^{(i)} x^j$, $q_i^{(i)} = 1$.

Algorithm 2

• Step 1 (Initialization): Choose an integer n and set $q_0^{(-1)} = q_{-1}^{(-1)} = 0$, $h_{-1} = 1$, $k_0 = -1$, $a_{-1} = 0$, $a_0 = c_n$, $q_0^{(0)} = 1$, $q_{-1}^{(0)} = 0$, $k = 0$, $\varepsilon_0^{(n-1)} = \sum_{i=0}^{n-1} c_i$.

• Step 2 (Determination of $\theta_n(k)$):
1 $i = 0$
2 $h_{k+i} = \sum_{j=0}^{k} (c_{n+k+i+j+1} - c_{n+k+i+j}) q_j^{(k)}$
if $|h_{k+i}| < tol$ for some tolerance tol, then

$i = i + 1$, go to 2
end (if)
$\theta_n(k) = k + i$
$d_{m-1} = \sum_{j=0}^{k} (c_{n+\theta_n(k)+m+j+1} - c_{n+\theta_n(k)+m+j}) q_j^{(k)}, \; m = 1, \ldots, i+1$

- STEP 3:

$b_k = a_k / h_{\theta_n(k)}$
for $i = k, \ldots, \theta_n(k)$
$\varepsilon_{2i+2}^{(n-1)} = \varepsilon_{2i}^{(n-1)} - b_k a_i$, $\alpha_i = q_{k-1}^{(i)} + (\sum_{j=k}^{i} d_{j-k} q_j^{(i)}) / h_{\theta_n(k)}$
$\beta_i = \sum_{j=0}^{i} (c_{n+j+k+1} - c_{n+j+k}) q_j^{(i)} / h_{k-1}$
$q_j^{(i+1)} = q_{j-1}^{(i)}, \quad j = 1, \ldots, i+1$
$q_j^{(i+1)} \leftarrow q_j^{(i+1)} - \alpha_i q_j^{(k)}, \quad j = 0, \ldots, k$
$q_j^{(i+1)} \leftarrow q_j^{(i+1)} - \beta_i q_j^{(k_0)}, \quad j = 0, \ldots, k_0$
$a_{i+1} = a_i - \alpha_i a_k - \beta_i a_{k_0}$
end (for)
if $k = 0$, then $a_{\theta_n(0)+1} = a_{\theta_n(0)+1} + (c_{n+\theta_n(0)+1} - c_{n+\theta_n(0)})$
end (if)
$k_0 = k$, $k = \theta_n(k) + 1$
go to 1
end.

Let us mention that Algorithm 2 can also be applied to sequences. If we want to apply it to a sequence $\{U_i\}_{i \in \mathbb{N}}$, then we set $c_0 = U_0$ and $c_i = U_i - U_{i-1}$ for $i > 0$.

6.1. *Numerical results*

EXAMPLE 1. We start by applying Algorithm 2 to the power series

$$\begin{aligned} f(t) = 1 &+ at + at^2 + \ldots + at^{m-1} \\ &+ t^m + at^{m+1} + at^{m+2} + \ldots + at^{2m-1} + t^{2m} + at^{2m+1} + \ldots \end{aligned}$$

which has been studied in [11]. This is the expansion of the rational function $(1 + at + at^2 + \ldots + at^{m-1})/(1 - t^m)$ for $t \in \,]-1, 1[$. In Example 2 of Subsection 5.3, we were interested in the computation of the coefficients of the Padé approximants. Now, we want to get an approximation of $f(t)$ for a fixed t by using Algorithm 2. We set $t = 0.9, a = 0.001$, $tol = 10^{-16}$, and $m = 7$. The exact value of $f(0.9)$ is $1.924882238575926\ldots$ By setting $c_i = at^i$ and applying Algorithm 2, we obtain

$\varepsilon_{2k}^{(0)}$	Algorithm 2
$\varepsilon_{0}^{(0)}$	0.1000000000000000D+01
$\varepsilon_{2}^{(0)}$	0.1009000000000000D+01
$\varepsilon_{4}^{(0)}$	0.1009000000000000D+01
$\varepsilon_{6}^{(0)}$	0.1009000000000000D+01
$\varepsilon_{8}^{(0)}$	0.1009000000000000D+01
$\varepsilon_{10}^{(0)}$	0.1009000000000000D+01
$\varepsilon_{12}^{(0)}$	0.9999745519928722D+00
$\varepsilon_{14}^{(0)}$	0.1924882238573816D+01

A true breakdown is avoided from iteration $k = 2$ to $k = 5$. As the power series f converges to a rational function and from the properties of the Padé approximants, we deduce that, in exact arithmetic, the sequence $\{\varepsilon_{2k}^{(0)}\}_k$ gives at the 7th iteration the exact value of $f(0.9)$. This explains that $\varepsilon_{14}^{(0)}$ gives us a good approximation of $f(0.9)$ by using Algorithm 2.

Example 2. Consider the power series $f(t) = \sum_{i=0}^{\infty} 4t^{5i}/(2i+1)$ which converges to the function S defined by

$$S(t) = \begin{cases} (4/\sqrt{t^5})\,\mathrm{arctanh}(\sqrt{t^5}) & \text{for } t \in \,]0,1[, \\ (4/\sqrt{-t^5})\,\arctan(\sqrt{-t^5}) & \text{for } t \in \,]-1,0[, \end{cases}$$

$$S(0) = 4, \qquad S(-1) = \pi = 3.14159265358979323846264 33\ldots$$

For $t = -1$, the application of Algorithm 2 to this power series with $tol = 10^{-14}$ gives the following results:

k	S_{2k-1}	$\varepsilon_{2k}^{(-1)}$ obtained by Algorithm 2
1	4.000	4.000000000000000
6	2.666	$\underline{3.1}66666666666667$
11	3.466	$\underline{3.14}2342342342341$
16	2.895	$\underline{3.141}614906832296$
21	3.339	$\underline{3.14159}3311879925$
26	2.976	$\underline{3.1415926}73030332$
31	3.283	$\underline{3.14159265}4163364$
36	3.017	$\underline{3.141592653}606703$
41	3.252	$\underline{3.1415926535}90289$
46	3.041	$\underline{3.1415926535897}91$

From these results, it is obvious that Algorithm 2 accelerates the convergence of the sequence $S_1 = 4$, $S_{11} = 4 - 4/3$, $S_{21} = 4 - 4/3 + 4/5, \ldots$ given by Leibniz to the exact value of π.

Acknowledgments. The author thanks Professor C. Brezinski for suggesting the problem, Professor J. Van Iseghem for many helpful comments and Professor H. Sadok for useful discussions.

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E. H. Ayachour
Laboratoire d'Analyse Numérique et d'Optimisation
UFR IEEA-M3
Université des Sciences et Technologies de Lille
59655 Villeneuve d'Ascq Cedex, France
E-mail: ayachour@ano.univ-lille1.fr

Received on 6.7.1998