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The Lanczos method and its variants can be used to solve efficiently the rational interpolation problem. In this paper we present a suitable fast modification of a general look-ahed version of the Lanczos process in order to deal with polynomials expressed in the Chebyshev orthogonal basis. The proposed approach is particularly suited for rational interpolation at Chebyshev points, that is, at the zeros of Chebyshev polynomials. In fact, in this case it overcomes some of the numerical difficulties which limited the applicability of the look-ahed Lanczos process for determining the coefficients both of the numerators and of the denominators with respect to the standard power basis.

1. Introduction

Developing numerical methods for computing approximations of analytic functions by means of polynomials and rational functions represents a fundamental research area of the computational mathematics. A customary approach which goes back to the classical 19th century analysis is based on the interpolation techniques. Recently, these techniques have been reviewed in order to combine numerical stability and efficiency and, in this respect, Chebyshev approximation have become a major computational tool.

Chebyshev polynomial approximation, that is, the approximation of a function $f(x)$ by means of a truncated Chebyshev expansion $\sum_{i=0}^{n} c_i T_i(x)$, where $T_i(x) = 2\cos(i \arccos(x/2)$ is the Chebyshev polynomial of degree i for the interval $[-2,2]$, can be accomplished in a fast and stable way if fast cosine transform methods are used. Reichel [18] proposed a fairly stable numerical scheme for the polynomial approximation of an analytic function $f(x)$ on a set K which generalizes Chebyshev approximation. Reichel's methods first scales K to have capacity 1 and then it computes the polynomial which interpolates $f(x)$ in a set of Leja points for K. In the case when K is an interval, $K = [-a, a]$, $a \geq 0$, K has capacity $a/2$ and therefore the first stage of Reichel's scheme amounts to shift K into the interval $[-2,2]$. Then, the Leja interpolation nodes are distributed roughly as the zeros of the Chebyschev polynomials.

Chebyshev rational function approximation methods which compute a rational ap-

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proximation $r_{m,n}(x)$ to $f(x)$,

$$r_{m,n}(x) = \frac{\sum_{i=0}^{m} a_i T_i(x)}{\sum_{i=0}^{n} b_i T_i(x)},$$

given the Chebyschev expansion $\sum_{i=0}^{+\infty} c_i T_i(x)$ of $f(x)$, are used both for approximating elementary functions [9], [4], and as a starting point for the second Remez algorithm that converges to the best rational approximation [17]. These methods proceed in the same manner as Padé approximation. The $m+n+1$ unknowns a_i and b_i are defined by as many conditions $r_j = 0$, $0 \le j \le m+n$, r_j being the coefficients of the Chebyshev expansion of the following function

$$\sum_{i=0}^{n} b_i T_i(x) \sum_{i=0}^{+\infty} c_i T_i(x) - \sum_{i=0}^{m} a_i T_i(x).$$

Performing the multiplications and applying the identity

$$T_{i+j}(x) + T_{i-j}(x) = T_i(x) T_j(x), \tag{1.1}$$

we obtain a system of linear equations which determines the unknowns a_i and b_i.

However, two problems arise with this approach. The first one involves the computation of the Chebyshev series for $f(x)$ since practically a numerical integration technique is required; the second one occours because the solution of the resulting linear systems apparently required $O((n+m)^3)$ arithmetical operations. Rational interpolation is a cheap alternative that obtains comparable results [14].

In this paper we will face the problem of finding the coefficients in the Chebyshev basis both of the numerators $p_m(x)$ and of the denominators $q_n(x)$ of all the existing rational functions $r_{m,n}(x) = p_m(x)/q_n(x)$ which assume given values $f_0, \ldots, f_N$ at the distinct Chebyshev points $x_i = \cos((2i+1)\pi/(2N+2))$, $0 \le i \le N$, $N = m+n$.

Our point of departure is represented by some modifications of the classical Jacobi's algorithm for rational approximation [15] which rely on the Lanczos process.

In the standard case where the polynomials are represented into power form, Lanczos algorithm can be seen into a matrix setting as a Levinson-type method for computing the upper triangular matrix R and the block diagonal matrix D which define a generalized triangular factorization of the inverse of an Hankel matrix H, that is, $R^T H R = D$. This block triangular factorization is not usually unique but, on the contrary, there are univocally determined the entries of the columns r_{m_i} of $R = (r_0, \ldots, r_N)$ where $0 = m_0 < m_1 < \ldots < m_l = N+1$ are the integers such that the $m_i \times m_i$ leading principal submatrix H_{m_i-1} of $H = H_N$ is nonsingular. If we introduce the polynomials

$$z_i(x) = (1, x, \ldots, x^N) r_{m_i},$$

then we find that they are orthogonal with respect to the symmetric bilinear form

$$\langle \phi, \psi \rangle = z^T H w, \ \phi(x) = (1, \ldots, x^N) z, \ \ \psi(x) = (1, \ldots, x^N) w.$$

Moreover, they satisfy a three-term recurrence relation,

$$z_{i+1}(x) = c_{i+1}(x) z_i(x) - b_i z_{i-1}(x), \quad z_{-1}(x) = 0, \quad z_0(x) = 1$$

where $c_i(x)$ are monic polynomials of degree $\delta_i = m_i - m_{i-1}$. In this way, by using the identity

$$\langle z_i(x), x z_j(x) \rangle = \langle x z_i(x), z_j(x) \rangle, \tag{1.2}$$

we are able to compute all of the coefficients of the polynomials $z_i(x)$ at the optimum computational cost of $O(N^2)$ arithmetical operations.

The modifications of the Jacobi's algorithm developed in [5] and [10] essentially consist of performing the Lanczos process in order to determine the block triangular factorizations of two Hankel matrices H_N and H'_N which are connected to the rational interpolation conditions in the following way:

$$H_N = VDV^T, \quad H'_N = VD'V^T$$

where $V = (x_j^{i-1})$ is the Vandermonde matrix with nodes x_j and D and D' are diagonal matrices with diagonal entries $d_i = f_i / \prod_{j=0, j\neq i}^{N}(x_i - x_j)$ and $d'_i = 1/(f_i \prod_{j=0, j\neq i}^{N}(x_i - x_j))$, respectively. The polynomials $z_i(x)$ and $z'_i(x)$ associated with the block triangular factorization of H_N and H'_N define, respectively, the denominators and the numerators of the wanted rational interpolating functions.

However, in finite precision arithmetic these methods suffer from potential instabilities which occur when polynomials $z_i(x)$ and $z'_i(x)$ corresponding to ill-conditioned leading principal sumatrices of H_N or H'_N are computed. On the other hand, it is possible to modify the Lanczos process so that it skips certain ill-conditioned leading submatrices, or, equivalently, it computes only a "well-conditioned" sequence of polynomials (see [6], [7]). Such look-ahed variants of the Lanczos process are generally fast, that is, they generally require $O(N^2)$ arithmetical operations if the number of ill-conditioned submatrices is independent of N. Nevertheless, the application of the look-ahed Lanczos process in the context of the rational interpolation problem is not straightforward. In fact, the Hankel matrices H_N and H'_N are tipically ill-conditioned already for small values of N and this implies that there are no moderate upper bounds for the condition munber of the $(N-k)\times(N-k)$ leading principal submatrix of H'_N in terms of the condition number of the $(k+1)\times(k+1)$ leading principal submatrix of H_N. Roughly speaking, this means that "well-conditioned" denominators do not necessarily correspond with "well-conditioned" numerators and vice versa.

Here, we first derive a suitable modification of a general look-ahed version of the Lanczos procedure [7] in order to compute the polynomials $z_i(x)$ in generalized form, that is, relative to a given orthogonal basis $\{l_i(x)\}$. By replacing the Hankel matrix H with the matrix $\hat{H} = LHL^T$ where L is the $(N+1)\times(N+1)$ lower triangular matrix whose $(i+1)$-st row is defined by the coefficients of the monic polynomial $l_i(x)$, then we find that

$$z_i(x) = (l_0(x), , \ldots, l_N(x))\hat{r}_{m_i},$$

where $\hat{r}_j$ are the columns of the upper triangular matrix $\hat{R}$ such that $\hat{R}^T\hat{H}\hat{R} = \hat{D}$. This implies that the polynomials $z_i(x)$ expressed in generalized form are orthogonal with respect to the symmetric bilinear form

$$\langle \phi, \psi \rangle = \hat{z}^T\hat{H}\hat{w}, \phi(x) = (l_0(x), \ldots, l_N(x))\hat{z}, \quad \psi(x) = (l_0(x), \ldots, l_N(x))\hat{w}.$$

In the case where $l_i(x) = T_i(x)$, that is, we are looking for polynomials expressed in the Chebyshev basis, it is computationally worth mentioning that, up to multiplication on the right and on the left by a suitable diagonal matrix, $\hat{H}$ belongs to an algebra of matrices which can be diagonalized by means of the cosine transform and, therefore, $O(N \log N)$ arithmetical operations are sufficient to evaluate the product of $\hat{H}$ by a vector in a stable way. Furthermore, since a somewhat more general formulation of the relation 1.2 still holds, then we may usually determine a suitable subsequence of the polynomials

$z_i(x)$ in generalized form, without at any stage converting polynomials into power form, at the computational cost of $O(N^2)$ arithmetical operations.

With respect to the stability issues, we observe that both $\hat{H}_N$ and $\hat{H'}_N$ are fairly well-conditioned matrices since their condition number depends only on the values f_i. This allows us to give a moderate upper bound for the condition number of $\hat{H'}_{N-k-1}$ in terms of the condition number of $\hat{H}_k$ which shows that $\hat{H'}_{N-k-1}$ is well-conditioned if and only if $\hat{H}_k$ is well-conditioned. In this way, our modification of the Lanczos process applied to $\hat{H'}_N$ computes the needed sequence of numerators in a stable way.

Some preliminary computational experience with this approach is the subject of the last section. We report a wide set of computed examples where the values f_i are either generated at random or they represent the values that an elementary function $f(x)$ assumes at the interpolation nodes x_i. In all of these cases, computational results are quite promising.

2. Jacobi's algorithm for polynomials represented in the Chebyshev basis

The Chebyshev polynomial of degree i, $i \geq 1$ on $[-2, 2]$ is denoted $T_i(x)$ and is given by the explicit formula

$$T_i(x) = 2\cos(i \arccos(x/2)).$$

By means of trigonometric identities, we obtain the following three-term recurrence relation

$$T_{i+1}(x) = xT_i(x) - \beta_i T_{i-1}(x), \quad T_{-1}(x) = 0, \quad T_0(x) = 1, \tag{2.1}$$

where $\beta_1 = 2$ and $\beta_i = 1$ if $i > 1$. Relation 2.1 says that $T_i(x)$ coincides with the characteristic polynomial of the tridiagonal matrix T_i,

$$T_i = \begin{pmatrix} 0 & 1 & & & \\ 2 & 0 & 1 & & \\ & 1 & 0 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & 0 \end{pmatrix}.$$

The polynomial $T_i(x)$ has i zeros $x_j^{(i)}$ in the interval $[-2, 2]$,

$$x_j^{(i)} = 2\cos(\frac{(2j+1)\pi}{2i}), \quad 0 \leq j \leq i-1$$

and, hereafter, we will refer to the set $\mathcal{C}_i = \{x_j^{(i)},\ j = 0, \ldots, i-1\}$ as to the $i-$th Chebyshev set. Finally, the polynomials $T_i(x)$ satisfy the following discrete orthogonality relations

$$\sum_{j=0}^{i-1} T_h(x_j^{(i)}) T_k(x_j^{(i)}) = \begin{cases} 0, & \text{if } h \neq k; \\ 2i, & \text{if } h = k \neq 0; \\ i, & \text{if } h = k = 0. \end{cases} \tag{2.2}$$

The Chebyshev rational interpolation problem at the Chebyshev set $\mathcal{C}_{N+1}$ is that of finding all of the rational functions $r_{m,n}(x)$, $N = m + n$,

$$r_{m,n}(x) = \frac{p_m(x)}{q_n(x)} = \frac{\sum_{i=0}^{m} a_i T_i(x)}{\sum_{i=0}^{n} b_i T_i(x)},$$

which assume given values $f_0, \ldots, f_N$ at the points $x_j^{(N+1)}$, $0 \le j \le N$. If $n = 0$, the problem is reduced to Chebyshev polynomial interpolation and the solution exists and is unique. For fixed m and n, a direct approach consists of finding the solution of the following linear system

$$p_m(x_j^{(N+1)}) - f_j q_n(x_j^{(N+1)}) = 0 \quad 0 \le j \le N. \tag{2.3}$$

Since we have $N+1$ homogeneous linear equations in $N+2$ unknowns, then a nontrivial solution always exists. However, if $p_m(x_j^{(N+1)}) = q_n(x_j^{(N+1)}) = 0$ for a certain j, then a solution of 2.3 is not necessarily a solution of the rational interpolation problem. The points $(x_j^{(N+1)}, f_j)$ for which

$$p_m(x_j^{(N+1)}) = f_j q_n(x_j^{(N+1)}), \quad r_{m,n}(x_j^{(N+1)}) := \lim_{x \to x_j^{(N+1)}} \frac{p_m(x_j^{(N+1)})}{q_n(x_j^{(N+1)})} \neq f_j$$

are called the unattainable points, and $(x_j^{(N+1)}, f_j)$, $0 \le j \le N$, becomes a degenerate configuration for the pair (m, n).

Now, let us assume that $(x_j^{(N+1)}, f_j)$, $0 \le j \le N$, are not a degenerate configuration for the given pair (m, n), $m + n = N$. Since we have

$$\frac{T_h(x_j^{(N+1)}) p_m(x_j^{(N+1)})}{\prod_{i=0, i\neq j}^{N}(x_j^{(N+1)} - x_i^{(N+1)})} = \frac{T_h(x_j^{(N+1)}) f_j q_n(x_j^{(N+1)})}{\prod_{i=0, i\neq j}^{N}(x_j^{(N+1)} - x_i^{(N+1)})},$$

then we obtain that

$$\sum_{j=0}^{N} \frac{T_h(x_j^{(N+1)}) p_m(x_j^{(N+1)})}{\prod_{i=0, i\neq j}^{N}(x_j^{(N+1)} - x_i^{(N+1)})} = \sum_{j=0}^{N} \frac{T_h(x_j^{(N+1)}) f_j q_n(x_j^{(N+1)})}{\prod_{i=0, i\neq j}^{N}(x_j^{(N+1)} - x_i^{(N+1)})}. \tag{2.4}$$

The left-hand side of 2.4 represents the leading coefficients of the polynomial interpolating the function $T_h(x)p_m(x)$ at the Chebyshev set $\mathcal{C}_{N+1}$ and this implies

$$\sum_{j=0}^{N} \frac{T_h(x_j^{(N+1)}) f_j q_n(x_j^{(N+1)})}{\prod_{i=0, i\neq j}^{N}(x_j^{(N+1)} - x_i^{(N+1)})} = 0 \tag{2.5}$$

if $0 \le h \le n-1$. Relation 2.5 yields

$$\sum_{j=0}^{N} \frac{T_h(x_j^{(N+1)}) f_j}{\prod_{i=0, i\neq j}^{N}(x_j^{(N+1)} - x_i^{(N+1)})} \sum_{k=0}^{n} b_k T_k(x_j^{(N+1)}) = 0, \quad 0 \le h \le n-1$$

or, equivalently,

$$\sum_{k=0}^{n} b_k \Big(\sum_{j=0}^{N} \frac{T_h(x_j^{(N+1)}) T_k(x_j^{(N+1)}) f_j}{\prod_{i=0, i\neq j}^{N}(x_j^{(N+1)} - x_i^{(N+1)})} \Big) = 0, \quad 0 \le h \le n-1 \tag{2.6}$$

If $\hat{H}_N$ denotes the $(N+1) \times (N+1)$ matrix which has entries

$$\hat{h}_{r,s} = \sum_{j=0}^{N} \frac{T_{r-1}(x_j^{(N+1)}) T_{s-1}(x_j^{(N+1)}) f_j}{\prod_{i=0, i\neq j}^{N}(x_j^{(N+1)} - x_i^{(N+1)})}, \quad 0 \le r,\ s \le N \tag{2.7}$$

then the linear system 2.6 can be written into matrix form as

$$\hat{H}_{n-1}(b_0, \ldots, b_{n-1})^T = -b_n(\hat{h}_{1,n+1}, \ldots, \hat{h}_{n,n+1})^T \tag{2.8}$$

where $\hat{H}_{n-1}$ denotes the $n \times n$ leading principal submatrix of $\hat{H}_N$.

Relation 2.7 implies that $\hat{H}_N$ can be factorized as $\hat{V} D \hat{V}^T$ where $\hat{V}$ is a Vandermonde-like matrix,

$$\hat{V} = \begin{pmatrix} T_0(x_0^{(N+1)}) & \dots & T_0(x_N^{(N+1)}) \\ T_1(x_0^{(N+1)}) & \dots & T_1(x_N^{(N+1)}) \\ \vdots & & \vdots \\ T_N(x_0^{(N+1)}) & \dots & T_N(x_N^{(N+1)}) \end{pmatrix} = \begin{pmatrix} 1 & \dots & 1 \\ 2\cos(\frac{\pi}{2N+2}) & \dots & 2\cos(\frac{(2N+1)\pi}{2N+2}) \\ \vdots & & \vdots \\ 2\cos(\frac{N\pi}{2N+2}) & \dots & 2\cos(\frac{N\pi(2N+1)}{2N+2}) \end{pmatrix},$$

and D is a diagonal matrix with diagonal entries

$$d_i = \frac{f_{i-1}}{\prod_{j=0, j\neq i-1}^{N}(x_{i-1}^{(N+1)} - x_j^{(N+1)})} = \frac{1}{N+1}(-1)^{i-1} f_{i-1} \sin(\frac{\pi(2i-1)}{2N+2}).$$

From the orthogonality conditions 2.2, we obtain that

$$\hat{V}\hat{V}^T = (N+1)S, \quad S = \begin{pmatrix} 1 & & & \\ & 2 & & \\ & & \ddots & \\ & & & 2 \end{pmatrix},$$

which says that $Q = \sqrt{N+1} S^{-1/2} V$ is a real orthogonal matrix and, therefore, $S^{-1/2}\hat{H}_N S^{-1/2}$ belongs to the matrix algebra generated over $\mathbf{R}$ by the matrix

$$\hat{T}_N = \begin{pmatrix} 0 & \sqrt{2} & & & \\ \sqrt{2} & 0 & 1 & & \\ & 1 & 0 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & 0 \end{pmatrix}.$$

This allows us to perform the multiplication of $\hat{H}_N$ by a vector at the cost of $O(N^2)$ arithmetical operations for any order N; moreover, if N is a power of two, then the fast cosine transform methods reach the bound of $(N \log N)$ arithmetical operations.

By looking carefully at the structure of the leading principal submatrices $\hat{H}_i$ of $\hat{H}_N$, it can be easily found that $\hat{H}_N = L H_N L^T$ where H_N is an Hankel matrix and L is the $(N+1) \times (N+1)$ lower triangular matrix whose $(i+1)$-st row is defined by the coefficients of the monic polynomial $T_i(x)$. Such matrices have been studied in [11] and [12]; since they are the inverses of Bezoutians represented in the generalized basis, they have been called Hankel matrices expressed in the generalized basis. In this way, relation 2.8 represents a modified Yule-Walker equation and so, the theory for the the matrices having the form of $\hat{H}_N$ reduces to the classical theory of formally orthogonal polynomials associated with a family of Hankel matrices. In particular, if we denote as $0 = m_0 < m_1 < \ldots < m_l = N+1$ the integers such that the $\hat{H}_{m_i - 1}$ is nonsingular, then we find that there exists an interpolating rational function $r_{m,n}(x) = p_m(x)/q_n(x)$, where $q_n(x)$ has degree n, if and only if $n = m_i$ for a certain $i \neq l$. Moreover, the polynomials $q_{m_i}(x)$, suitably normalized in order to have leading coefficient equal to one, satisfy a three-term recurrence relation

$$q_{m_{i+1}}(x) = c_{i+1}(x) q_{m_i}(x) - d_i q_{m_{i-1}}(x), \quad q_{m_{-1}}(x) = 0, \; q_0(x) = 1$$

where $c_i(x)$ are monic polynomials of degree $\delta_i = m_i - m_{i-1}$,

$$c_i(x) = T_{\delta_i}(x) + \sum_{j=0}^{\delta_i - 1} c_{i,j} T_j(x).$$

Finally, if we consider the following symmetric bilinear form

$$\langle \phi, \psi \rangle = \hat{z}^T \hat{H}_N \hat{w}, \phi(x) = (T_0(x), \ldots, T_N(x))\hat{z}, \quad \psi(x) = (T_0(x), \ldots, T_N(x))\hat{w}, \tag{2.9}$$

we find that

$$\langle q_{m_i}, q_{m_j} \rangle \neq 0 \ \text{ if and only if } m_i = m_j .$$

The computation of the coefficients of the polynomials $q_{m_i}(x)$ expressed into power form by imposing the orthogonality conditions with respect a symmetric bilinear form is the core of the classical Lanczos process. In the following we will present a suitable generalization of the look-ahed Lanczos process of [7] for computing either the sequence $\{q_{m_i}(x)\}$ or a subsequence $\{q_{m_{i_k}}(x)\}$ of "well-conditioned" polynomials represented in the Chebyshev basis.

The algorithm generates a sequence of polynomials $\{q_i(x)\}$ where $q_i(x) = (T_0(x), \ldots, T_N(x))q_i$ is a monic polynomial of degree i. Adopting the notations introduced in [7], we denotes as $0 = \tilde{m}_0 < \tilde{m}_1 < \ldots < \tilde{m}_k = N + 1$ the integers such that $q_{\tilde{m}_i}(x) = q_{m_j}(x)$ for a certain j and $q_{\tilde{m}_i}(x)$ is computed by the algorithm. The polynomials $q_{\tilde{m}_i}(x)$ are called regular; the remaining polynomials are called inner. The polynomials $q_i(x)$ could be divided into k groups

$$\Phi^{(i)} = [q_{\tilde{m}_i}(x), \ldots, q_{\tilde{m}_{i+1}-1}(x)], \quad 0 \leq i \leq k-1$$

where the first polynomial is regular, while the remaining polynomials are inner polynomials. Moreover, if we set

$$\langle \Phi^{(i)}, \Phi^{(j)} \rangle = \begin{pmatrix} \langle q_{\tilde{m}_i}, q_{\tilde{m}_j} \rangle & \cdots & \langle q_{\tilde{m}_i}, q_{\tilde{m}_{j+1}-1} \rangle \\ \vdots & & \vdots \\ \langle q_{\tilde{m}_{i+1}-1}, q_{\tilde{m}_j} \rangle & \cdots & \langle q_{\tilde{m}_{i+1}-1}, q_{\tilde{m}_{j+1}-1} \rangle \end{pmatrix},$$

then the following block orthogonality conditions will be proved

$$\langle \Phi^{(i)}, \Phi^{(j)} \rangle = \begin{cases} 0, & \text{if } i \neq j; \\ \delta^{(i)}, & \text{if } i = j, \end{cases} \tag{2.10}$$

where $\delta^{(i)}$ is a nonsingular $(\tilde{m}_{i+1} - \tilde{m}_i) \times (\tilde{m}_{i+1} - \tilde{m}_i)$ matrix.

The look-ahed Lanczos process for polynomials expressed in generalized form proceeds as follows.

Algorithm 1

1 Initialize $q_0(x) = 1$, $\Phi^{(-1)} = \emptyset$, $\Phi = [q_0(x)]$, $i = 0$, $\tilde{m}_0 = 0$.
2 Decide whether to construct $q_{j+1}(x)$ as regular or inner polynomial and go to 3 or 4, respectively.
3 Set $\Phi^{(i)} = \Phi$. Compute

$$\alpha_j = (\delta^{(i)})^{-1} \langle \Phi^{(i)}, T_N^T q_j \rangle, \ \beta_j = (\delta^{(i-1)})^{-1} \langle \Phi^{(i-1)}, T_N^T q_j \rangle, \tag{2.11}$$

$$q_{j+1} = T_N^T q_j - \Phi^{(i)} \alpha_j - \Phi^{(i-1)} \beta_j . \tag{2.12}$$

Set $i = i + 1$, $\Phi = \emptyset$ and go to 5.

4 Compute

$$\beta_j = (\delta^{(i-1)})^{-1} \langle \Phi^{(i-1)}, T_N^T q_j \rangle, \tag{2.13}$$

$$q_{j+1} = T_N^T q_j - \Phi^{(i-1)} \beta_j. \tag{2.14}$$

5 Set $\Phi = [\Phi,\ q_{j+1}(x)]$.

Now, we will prove some basic properties of the algorithm. First we obtain a somewhat more general formulation of the relation 1.1.

PROPOSITION 2.1. *Let $\phi(x) = (T_0(x), \ldots, T_N(x))\phi$ and $\psi(x) = (T_0(x), \ldots, T_N(x))\psi$ be two polynomials of degree less than $N + 1$; then the relation*

$$\langle \phi, T_N^T \psi \rangle = \langle T_N^T \phi, \psi \rangle$$

holds.

Proof. From $T_N = S^{1/2} \hat{T}_N S^{-1/2}$ it follows that $T_N = V \Lambda V^{-1}$ where Λ is the diagonal matrix which has entries $\lambda_{i,i} = x_{i-1}^{(N+1)}$. Hence, we find that

$$\hat{H}_N T_N^T = V D V^T V^{-T} \Lambda V^T = V \Lambda D V^T = T_N \hat{H}_N.$$

Now, we are able to show that the polynomials $q_j(x)$ generated by the above algorithm satisfy the block orthogonal conditions 2.10 with respect to the symmetric bilinear form 2.9.

PROPOSITION 2.2. *If $\tilde{m}_i \leq j \leq \tilde{m}_{i+1} - 1$, then we have*

$$\langle \Phi^{(s)}, q_{j+1} \rangle = 0, \quad s = 0, \ldots, i' \tag{2.15}$$

where $i' = i - 1$ if $q_{j+1}(x)$ is a inner polynomial and, otherwise, $i' = i$ if $q_{j+1}(x)$ is a regular polynomial. Moreover, if $q_{j+1}(x)$ is a regular polynomial, then q_{j+1} satisfies the equation 2.8 with $n = \tilde{m}_{i+1}$ and, finally, we find that

$$\delta^{(i)} = \langle \Phi^{(i)}, \Phi^{(i)} \rangle \text{ is nonsingular.} \tag{2.16}$$

Proof. In view of Proposition 2.1, the proofs of 2.15 and 2.16 follow with some minor adaptations from that of Theorem 2.3 of [7] for the standard power form case. Now let us assume that $q_{j+1}(x)$ is a regular polynomial of degree $\tilde{m}_{i+1}$. The block orthogonality relations 2.10 implies that x^h, $0 \leq h \leq m_{i+1} - 1$, is orthogonal to $q_{j+1}(x)$ and, therefore, there follows that q_{j+1} satisfies equation 2.8 with $n = \tilde{m}_{i+1}$.

To determine the number of arithmetical operations required for Algorithm 1 we count the operations at each step. The computation of q_{j+1} by means of 2.12 or 2.14 can be performed in $O(N + (\tilde{m}_{i+1} - \tilde{m}_i)^2 + (\tilde{m}_i - \tilde{m}_{i-1})^2)$ arithmetical operations. Concerning the computation of α_j and β_j at stage 2 and 3, we observe that it can be reduced to solve linear systems with coefficient matrices $\delta^{(h)}$ of size $(\tilde{m}_{h+1} - \tilde{m}_h) \times (\tilde{m}_{h+1} - \tilde{m}_h)$. By using Proposition 2.1 we can also compute the vectors $\langle \Phi^{(i)}, T_N^T q_j \rangle$ and $\langle \Phi^{(i-1)}, T_N^T q_j \rangle$

at the cost of $O(N(\tilde{m}_{i+1} - \tilde{m}_i)(\tilde{m}_i - \tilde{m}_{i-1}))$ and $O(N(\tilde{m}_i - \tilde{m}_{i-1})^2)$, respectively. This means that we may determine α_j and β_j at stage 2 and 3 of Algorithm 1 at the cost of $O(N\delta^2 + \delta^3)$ arithmetical operations where $\delta = \max_i(\tilde{m}_i - \tilde{m}_{i-1})$.

Criteria for skipping certain polynomials in the Lanczos process or, equivalently, certain leading principal submatrices in the fast Hankel and Toeplitz system solvers have been proposed before by several authors [7], [13], [1], [3] and [2]. The implementation of these tests, which can easily generalized for the matrix $\hat{H}_N$, usually require less than $O(\delta^3)$ arithmetical operations. Since δ is tipically $O(1)$, the cost of Algorithm 1 is $O(N^2)$ but it can increase in certain pathological cases.

In this way, we finally arrive at the following direct algorithm for rational interpolation at Chebyshev points. This algorithm algorithm is essentially a modification of that of [7] in order to manipulate polynomials in generalized form without converting polynomials into power form at any stage.

Algorithm 2
Input: $(x_j^{(N+1)}, f_j)$, $f_j \neq 0$, $0 \leq j \leq N$.
Output: coefficients of the polynomials $q_{\tilde{m}_i}(x)$ and $p_{N-\tilde{m}_i}(x)$ in the Chebyschev basis.

1 Compute the coefficients of $q_{\tilde{m}_i}(x)$ in the Chebyschev basis by means of Algorithm 1.
2 Compute the coefficients of $\hat{p}_{N-\tilde{m}_i}(x)$ in the Chebyschev basis by using Algorithm 1 on the data set $(x_j^{(N+1)}, f_j^{-1})$, $0 \leq j \leq N$, with an a priori fixed sequence of jumps, i.e., without performing stage 2 of Algorithm 1 at any step.
3 Set $p_{N-\tilde{m}_i}(x) = \gamma_i \hat{p}_{N-\tilde{m}_i}(x)$, where γ_i is such that

$$\frac{q_{\tilde{m}_i}(x_j^{(N+1)})}{\hat{p}_{N-\tilde{m}_i}(x_j^{(N+1)})} f_j = \gamma_i$$

for $(x_j^{(N+1)}, f_j)$ attainable point.

The complexity of this algorithm is generally $O(N^2)$ arithmetical operations. Its correctness relies on the following result. We denote as $||A||$ the Euclidean norm of the matrix A and $\mathcal{K}(A)$ is the corresponding Euclidean condition number.

PROPOSITION 2.3. *Let us denote as $\hat{H}'_N$ the matrix $\hat{V}D'\hat{V}^T$ where D' is a diagonal matrix with diagonal entries*

$$d'_i = (f_{i-1} \prod_{j=0, j\neq i-1}^{N} (x_{i-1}^{(N+1)} - x_j^{(N+1)}))^{-1}.$$

Moreover, assume that $\hat{H}_N$ is partitioned as follows

$$\hat{H}_N = \begin{pmatrix} \hat{H}_k & A \\ A^T & B \end{pmatrix}.$$

Then $\hat{H}_k$ is nonsingular if and only if the $(N-k) \times (N-k)$ leading principal submatrix

$\hat{H}'_{N-k-1}$ of $\hat{H}'_N$ is nonsingular. Further, if $\hat{H}_k$ is nonsingular, we have

$$\mathcal{K}(\hat{H}'_{N-k-1}) \leq 2(N+1)^2\rho^2 \frac{\max_j |f_j \sin(\frac{\pi(2j-1)}{2N+2})|}{\min_j |f_j \sin(\frac{\pi(2j-1)}{2N+2})|}(\frac{\max_j \sin(\frac{\pi(2j-1)}{2N+2})}{\min_j \sin(\frac{\pi(2j-1)}{2N+2})})^2$$

where

$$\rho = 1 + (\frac{||A||\mathcal{K}(\hat{H}_k)}{||\hat{H}_k||})^2.$$

Proof. First of all, we observe that if $v(x)$ and $w(x)$ are the interpolating polynomials at the data set $(x_j^{(N+1)}, f_j)$ and $(x_j^{(N+1)}, 1/f_j)$, respectively, then they satisfy the Bezout's equality

$$w(x)v(x) = 1 \ (\mod \ T_{N+1}(x)).$$

Hence, generalizing a standard property which relates Hankel and Bezout matrices (see, e.g., Th. 6.3 of [8]), one readily obtains that

$$\hat{H}'_N B \hat{H}_N B^T = I_N \tag{2.17}$$

where I_N denotes the $(N+1)\times(N+1)$ identity matrix. The matrix B, which appears in 2.17, satisfies $B = \hat{V}^{-T}\tilde{D}\hat{V}^{-1}$ where $\tilde{D}$ is a diagonal matrix such that

$$\tilde{d}_i = \prod_{j=0, j\neq i-1}^{N} (x_{i-1}^{(N+1)} - x_j^{(N+1)})^{-1} = \frac{(-1)^{i-1}}{N+1}\sin(\frac{\pi(2i-1)}{2N+2}).$$

Moreover, if J_N denotes the $(N+1)\times(N+1)$ permutation matrix which has its antidiagonal entries equal to 1, then we find that $J_N B$ is a lower triangular matrix. Now, assume that the $(k+1)\times(k+1)$ leading principal submatrix $\hat{H}_k$ is nonsingular, then the block factorization formula

$$\hat{H}_N = \begin{pmatrix} \hat{H}_k & A \\ A^T & B \end{pmatrix} = \begin{pmatrix} I_k & 0 \\ \hat{H}_k^{-1}A & I_{N-k-1} \end{pmatrix} \begin{pmatrix} \hat{H}_k & 0 \\ 0 & \Gamma \end{pmatrix} \begin{pmatrix} I_k & A^T\hat{H}_k^{-1} \\ 0 & I_{N-k-1} \end{pmatrix} \tag{2.18}$$

holds. Since $\hat{H}_N$ is nonsingular, there follows that Γ is a nonsingular $(N-k)\times(N-k)$ matrix. By combining the equality $J_N J_N = I_N$ with relation 2.17 we obtain that

$$J_N \hat{H}'_N J_N J_N B \hat{H}_N B^T J_N = I_N$$

which gives

$$J_N \hat{H}'_N J_N = J_N B^{-T} \hat{H}_N^{-1} B^{-1} J_N = B^{-T} J_N J_N \hat{H}_N^{-1} J_N J_N B^{-1}. \tag{2.19}$$

Relation 2.18 and 2.19 imply that the matrix $\hat{H}'_N$ can be written in the form

$$(J_N B)^{-1} J_N \begin{pmatrix} I_k & -A^T\hat{H}_k^{-1} \\ 0 & I_{N-k-1} \end{pmatrix} \begin{pmatrix} \hat{H}_k^{-1} & 0 \\ 0 & \Gamma^{-1} \end{pmatrix} \begin{pmatrix} I_k & 0 \\ -\hat{H}_k^{-1}A & I_{N-k-1} \end{pmatrix} J_N (J_N B)^{-T}$$

which, finally, yields

$$\hat{H}'_{N-k-1} = ((J_N B)^{-1})_{N-k-1} J_{N-k-1} \Gamma^{-1} J_{N-k-1} ((J_N B)^{-T})_{N-k-1}. \tag{2.20}$$

Relation 2.20 shows that $\hat{H}_k$ is nonsingular if and only if $\hat{H}'_{N-k-1}$ is nonsingular. Furthermore, it can be used for estimating the Euclidean condition number of the matrix

$\hat{H}'_{N-k-1}$. In fact, by means of 2.18, it is easy to verify that

$$\mathcal{K}(\Gamma) \leq \rho^2 \mathcal{K}(\hat{H}_N) \tag{2.21}$$

where

$$\rho = 1 + (\frac{||A||\mathcal{K}(\hat{H}_k)}{||\hat{H}_k||})^2.$$

Since $S^{-1/2}\hat{H}_N S^{-1/2} = QDQ^T$ where Q is a real orthogonal matrix, then we find that

$$\mathcal{K}(\hat{H}_N) \leq 2\frac{\max_j |f_j \sin(\frac{\pi(2j-1)}{2N+2})|}{\min_j |f_j \sin(\frac{\pi(2j-1)}{2N+2})|}. \tag{2.22}$$

Finally, since $J_N B$ is a lower triangular matrix, we can prove that

$$\mathcal{K}((J_N B)^{-1})_{N-k-1}) \leq (N+1)\frac{\max_j \sin(\frac{\pi(2j-1)}{2N+2})}{\min_j \sin(\frac{\pi(2j-1)}{2N+2})} \tag{2.23}$$

and, hence, by combining relations 2.20, 2.21 and 2.22, we conclude the proof.

Proposition 2.3 gives a moderate upper bound for the condition number of $\hat{H}'_{N-k-1}$ in terms of the condition number of $\hat{H}_k$; it is worth mentioning that no acceptable upper bounds can be formulated in the standard case when polynomials are represented into power form since Hankel and Bezout matrices are tipically ill-conditioned already for small values of N.

In the next section, we discuss an implementation of Algorithm 2 and we report the results of numerical experiments.

3. Computational Results

Computational results for the above described approach are quite promising but are certainly preliminary. There are in fact many numerical issues that should be addressed and, at present, we have concentrated our attention only on a few of them. We have implemented two versions of Algorithm 2 in Fortran and we have made numerical experiments on a computer with machine precision of order 10^{-15}.

We have first investigated the behaviour of Algorithm 2 when the values f_i at the interpolation nodes are generated at random. In this case all of the leading principal submatrices of $\hat{H}_N$ and $\hat{H}'_N$ are generally nonsingular but, however, if we solve a linear system defined by a ill-conditioned leading principal submatrix then poor results can be expected. In order to check the accuracy of the computed rational interpolating functions, we have produced a version of Algorithm 2 which uses the very simple criterion proposed by Sweet [19] for skipping singular leading principal submatrices. The decision for taking a block step is based on the so-called prediction error which is zero if and only if the corresponding leading principal submatrices is singular. In finite precision arithmetic, we perform a block step when the prediction error is less than a fixed threshold-value. Our implementations use the threshold-value 10^{-12}. Of course, an ill-conditioned leading principal submatrix is not guaranteed to be revealed by a small prediction error and, therefore, the resulting algorithm is not numerically stable. This test is indeed not reliable for Hankel matrices.

We have considered 4 sets of numerical examples and, for each set, we generated 100

vectors $f_j = (f_{1,j}, \ldots, f_{50,j})^T$ which give the values of the rational interpolating functions at the interpolation nodes $x_i^{(49)} = \cos((2i-1)\pi/100)$, $1 \le i \le 50$. The index j is used as a counter for the 100 matrices.

1 This test set consists of vectors f_j with entries uniformly distributed in the interval $[0, 1]$. The uniform random deviates $f_{i,j}$ are generated by the function RAN1 of [16].

2 This test set consists of vectors f with entries $f_{i,j}$, $1 \le i \le 25$, generated by the function RAN1 of [16]. The vector f is completed by imposing the conditions $f_{50-i+1,j} = f_{i,j}$, $1 \le i \le 25$. Such "even" vectors produce matrices $\hat{H}_{49}$ and $\hat{H}'_{49}$ with leading principal submatrices of order $2k-1$ which are singular. Moreover, both the numerators and the denominators of the rational interpolating functions can be expressed in a sum involving Chebyshev polynomials of even degree. Our implementation uses these informations by computing the non-zero coefficients only.

3 This test set consists of vectors f_j with entries normally distributed with zero mean and unit variance. The random deviates $f_{i,j}$ with normal distribution are generated by the function GASDEV of [16].

4 This test set consists of vectors f with entries $f_{i,j}$, $1 \le i \le 25$, generated by the function GASDEV of [16]. The vector f_j is completed by imposing the conditions $f_{50-i+1,j} = f_{i,j}$, $1 \le i \le 25$. Again, the above described properties for "even" vectors are used.

For each pair $\hat{H}_{49}$, $\hat{H'}_{49}$, we solved the linear systems

$$\hat{H}_{49}x = (0, \ldots, 0, 1)^T, \quad \hat{H'}_{49}x' = (0, \ldots, 0, 1)^T$$

in a stable way by inverting the matrices $S^{-1/2}\hat{H}_{49}S^{-1/2}$ and $S^{-1/2}\hat{H'}_{49}S^{-1/2}$ which are diagonalized by the matrix Q. The relative errors ϵ_j and ${\epsilon'}_j$ are defined as

$$\epsilon_j = \frac{||x_j - r_j||_\infty}{||x_j||_\infty}, \quad \epsilon' = \frac{||{x'}_j - {r'}_j||_\infty}{||{x'}_j||_\infty}$$

where r_j and ${r'}_j$ are suitable columns of the computed upper triangular factors of the block triangular factorization of $\hat{H}_{49}$ and $\hat{H'}_{49}$, respectively. The absolute error η_j is defined as the maximum of the absolute errors

$$|r_{m,n}(x_i^{(49)}) - f_{i,j}|, \quad 1 \le i \le 50,$$

over all of the computed rational interpolating functions $r_{m,n}(x)$. For each test set, we consider the average errors

$$\epsilon = \frac{\sum_{j=1}^{100} \epsilon_j}{100}, \quad \epsilon' = \frac{\sum_{j=1}^{100} {\epsilon'}_j}{100}, \quad \eta = \frac{\sum_{j=1}^{100} \eta_j}{100}.$$

Table 1 below reports the results of our computations.

Table 1			
Test Set	ϵ	ϵ'	η
1	$3.5\ 10^{-9}$	$8.1\ 10^{-9}$	$4.8\ 10^{-5}$
2	$6.7\ 10^{-9}$	$3.7\ 10^{-9}$	$2.4\ 10^{-6}$
3	$1.0\ 10^{-7}$	$6.9\ 10^{-8}$	$5.0\ 10^{-5}$
4	$4.3\ 10^{-9}$	$9.1\ 10^{-9}$	$2.1\ 10^{-6}$

Table 1 shows that all of the leading principal submatrices of both $\hat{H}_{49}$ and $\hat{H'}_{49}$ are fairly well-conditioned in the average.

Afterwards, we have used rational interpolation at Chebyshev points for approximating even functions in the interval $[-2,2]$. We have considered 3 functions $f_j(x)$, $j = 1,2,3$, (j is here a counter for the approximated functions):

$$1\ \ f_1(x) = \frac{\log(4-x^2)}{\log(4+x^2)};$$
$$2\ \ f_2(x) = \frac{\arcsin(\sqrt{|x/2|}}{\sqrt{|x/2|}};$$
$$3\ \ f_3(x) = \frac{\arctan(\cos(2\ x))}{\cos(2\ x)}.$$

For each function, we have defined the vector $f_j = (f_{1,j}, \ldots, f_{32,j})^T$ as $f_{i,j} = f_j(x_i^{(31)})$, where $x_i^{(31)} = \cos((2i-1)\pi/64)$, $1 \le i \le 32$. Since, clearly, f_j are "even" vectors, then the algorithm computes only the non-zero coefficients both of the numerators and of the denominators of the rational approximations. Moreover, it applies Sweet's criterion to the leading principal submatrices of even order by using the threshold-value 10^{-12}. The error $|f_j(x) - r_{m,n}(x)|$ is evalueted at 38 equidistant points z_i in the interval $[-2,2]$, $z_i = -2 + (4/39)i$, $1 \le i \le 38$. We denote this seminorm by $||f_j(x) - r_{m,n}(x)||_d$ and we define the absolute error $\epsilon_{m,n,j}$ as $\epsilon_{m,n,j} = ||f_j(x) - r_{m,n}(x)||_d$. The absolute error η_j is defined as the maximum of the absolute errors

$$|r_{m,n}(x_i^{(31)}) - f_j(x_i^{(31)})|, \quad 1 \le i \le 32,$$

over all of the computed rational interpolating functions $r_{m,n}(x)$. Finally, we denote as $\max_{m,n}\epsilon_{m,n,j}$ and as $\min_{m,n}\epsilon_{m,n,j}$, respectively, the maximum and the minimum of $\epsilon_{m,n,j}$ over all of the pairs (m,n) such that the algorithm computes the rational function $r_{m,n}(x)$ which interpolates $f_j(x)$.

Table 2 below reports our computational results.

Table 1			
	$\max_{m,n}\epsilon_{m,n,j}$	$\min_{m,n}\epsilon_{m,n,j}$	η
1	$\epsilon_{0,30,1} = 101.6$	$\epsilon_{10,20,1} = 4.4\ 10^{-7}$	$3.7\ 10^{-5}$
2	$\epsilon_{2,28,2} = 6.0\ 10^{-3}$	$\epsilon_{18,12,2} = 6.5\ 10^{-4}$	$1.0\ 10^{-5}$
3	$\epsilon_{20,10,3} = 1.7\ 10^{-2}$	$\epsilon_{26,4,3} = 5.1\ 10^{-6}$	$1.6\ 10^{-2}$

The figures 1, 2 and 3, shown below, represent the error function

$$\log_{10}(|f_j(x) - r_{\bar{m},\bar{n},j}(x)|),$$

respectively, for $j = 1, 2, 3$, where $r_{\bar{m},\bar{n},j}(x)$ is such that $\epsilon_{\bar{m},\bar{n},j} = \min_{m,n} \epsilon_{m,n,j}$.

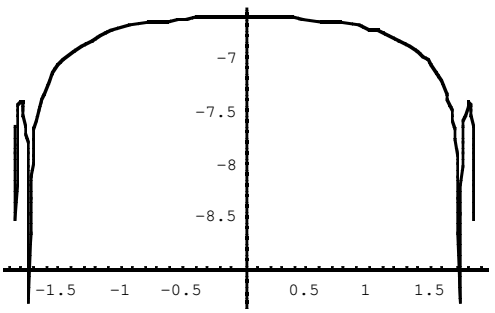


Fig. 1

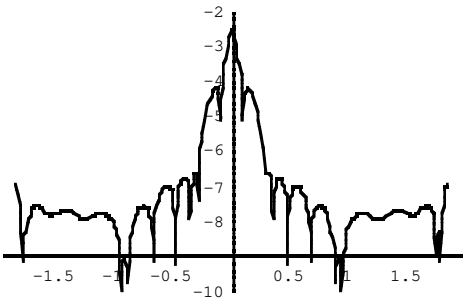


Fig. 2

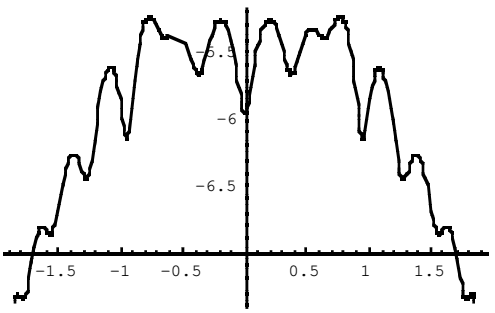


Fig. 3

It seems that this is quite a promising approach. However, in the case where the

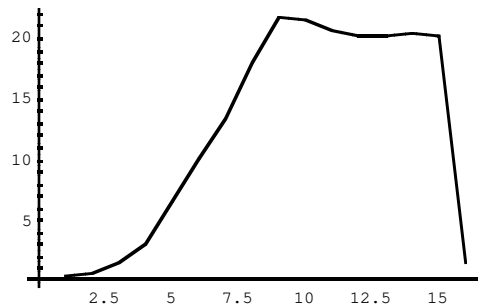
entries of the vector f represent the values which a function assumes at the interpolation nodes, our experience indicates that the matrices $\hat{H}_N$ and $\hat{H'}_N$ may have many ill-conditioned leading principal submatrices. For instance, when we apply our algorithm for approximating the function $f(x) = \arctan(x)/x$ on the interval $[-2+\sqrt{3}, 2-\sqrt{3}]$ by means of interpolation on the set $\mathcal{C}_8$, then we obtain very good results (the rational function $r_{\tilde{m},\tilde{n}}(x)$ such that $\epsilon_{\tilde{m},\tilde{n}} = \max_{m,n} \epsilon_{m,n}$ is

$$r_{1,4}(x) = \frac{12.0919 + 6.2235\ x}{12.0919 + 10.2539\ x^2 + x^4}$$

which is very close to the best rational function approximation

$$r_{1,4}(x) = \frac{12.0717 + 6.2180\ x}{12.0717 + 10.2419\ x^2 + x^4}).$$

If we increase the value of n and we consider rational interpolation on the set $\mathcal{C}_{32}$, we find a matrix $\hat{H}_{32}$ with the following condition number profile (we plot the logarithm to base 10 of the Euclidean condition number of the leading principal submatrices of even order).



A criterion for choosing the value of n is therefore required. At present, ad hoc choices are made and there is little understanding of the relation between the eigenvalue distribution of the leading principal submatrices of $\hat{H}_N$ and the function $f(x)$ that we would approximate. These investigations are under way and will be the topic of subsequent papers.

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