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LOOK-AHEAD LEVINSON- AND SCHUR-TYPE RECURRENCES IN THE PADÉ TABLE*

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Dedicated to Professor W. Niethammer on the occasion of his 60th birthday.

Abstract. For computing Padé approximants, we present presumably stable recursive algorithms that follow two adjacent rows of the Padé table and generalize the well-known classical Levinson and Schur recurrences to the case of a nonnormal Padé table. Singular blocks in the table are crossed by look-ahead steps. Ill-conditioned Padé approximants are skipped also. If the size of these look-ahead steps is bounded, the recursive computation of an (m, n) Padé approximant with either the look-ahead Levinson or the look-ahead Schur algorithm requires $O(n^2)$ operations. With recursive doubling and fast polynomial multiplication, the cost of the look-ahead Schur algorithm can be reduced to $O(n \log^2 n)$.

Key words. Padé approximation, Toeplitz matrix, Levinson algorithm, Schur algorithm, look-ahead, fast algorithm, biorthogonal polynomials, Szegő polynomials.

AMS subject classifications. 41A21, 42A70, 15A06, 30E05, 60G25, 65F05, 65F30.

1. Introduction.

It is well known that the computation of a Padé approximant[1] $r = p/q$ requires essentially the solution of a linear Hankel or Toeplitz system, which yields the coefficients of the denominator polynomial q. On the other hand, the recursive solution of such a system is linked to the computation of a finite sequence of Padé forms and Padé approximants. In particular, the leading principal submatrices of the Hankel matrix for computing the denominator of the (m, n) Padé approximant are the Hankel matrices of the linear systems for computing the Padé approximants that lie in the Padé table farther up on the same diagonal. If we flip around the coefficient vector and the columns of the Hankel matrix, we obtain a Toeplitz system. Then the leading principal submatrices correspond to the Padé approximants to the left of the (m, n) entry in the mth row of the Padé table. Therefore, certain recursive algorithms for computing Padé approximants follow a particular diagonal or row of the table. Other algorithms follow a staircase consisting of two adjacent diagonals or a sawtooth consisting of two adjacent rows. These recursive algorithms for Hankel or Toeplitz systems require typically $O(n^2)$ operations and, hence, are said to be fast. But some of them can be reformulated as recursive doubling methods and can make use of fast polynomial multiplication. Then the complexity reduces to $O(n \log^2 n)$ operations; Bitmead and Anderson [5], Brent, Gustavson, and Yun [6], Morf [28], Musicus [29], de Hoog [14], Ammar and Gragg [2, 1, 3] were the first to present such superfast algorithms.

The classical algorithm of Levinson (or Levinson-Durbin) [26, 16] is one that generates implicitly the denominators q of the Padé approximants on two adjacent rows, and it does this in a particular symmetric way. The Schur (or Schur-Bareiss) algorithm [32, 4] constructs the numerators p and the residuals e (defined below) of

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[1] We use the common term "Padé approximant" although "Padé interpolant" or "Padé fraction" would be more appropriate.

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the same Padé approximants. These classical versions of the Levinson and the Schur algorithm assume that the relevant Toeplitz matrix is Hermitian positive definite, and then the same holds for all leading principal submatrices. The two algorithms are easily adapted to the non-Hermitian case, but they still require that all the leading principal submatrices be nonsingular. Analogous assumptions are made in many other algorithms and in the papers cited above on superfast versions.

In the last ten years a number of more general algorithms have been derived that can deal with exactly singular submatrices; see Delsarte, Genin, and Kamp [15] for the indefinite Hermitian Toeplitz case, and Heinig [24, 25], Gover and Barnett [18], Sugiyama [33], Pombra, Lev-Ari, and Kailath [31], Tyrtyshnikov [37], and Pal and Kailath [30] for the non-Hermitian Toeplitz case. However, the so modified algorithms remain unstable when near-singular principal submatrices occur, and thus they are in practice limited to exact arithmetic, where they may still lead to very large intermediate quantities causing high memory needs, however. Only recently, numerically stable fast algorithms that can treat near-singular principal submatrices have been designed; for the Toeplitz case, see Sweet [34, 35], Chan and Hansen [11, 10, 12, 23], Freund and Zha [17], Gutknecht [20], and Gutknecht and Hochbruck [22, 21]. In this paper we translate the algorithms from [22], which were derived in a linear-algebra setting, into recurrences for Padé forms. We also give (often simpler) Padé theory based proofs instead of linear algebra proofs. In contrast to the recurrences introduced in [20], those presented here reduce in the case where all the relevant submatrices are well-conditioned exactly to the non-Hermitian versions of the algorithms of Levinson and Schur. As in the sawtooth algorithms of [20], the basic idea is to follow two adjacent rows of the Padé table and to jump over singular blocks. However, while the sawtooth algorithms make use of well-regular Padé forms, the algorithms derived here make use of well-column-regular Padé forms; see §3 and §6 for definitions. In contrast to the sawtooth recurrence, it can happen here that one has to jump over several well-conditioned blocks at once. Hence, in general the step size is larger than in the sawtooth algorithms. But, in practice, this drawback is hardly ever encountered, since look-ahead steps are relatively rare.

The paper is organized as follows. In Section 2 we introduce the notation and review the definition and some basic properties of the one-sided Padé approximation of a Laurent series. Section 3 is concerned with column-regular Padé forms, which play a fundamental role in look-ahead Levinson and Schur algorithms. Section 4 deals with two-point Padé forms. In particular, several equivalent definitions of column-regular two-point Padé forms are given, and it is shown how to compute them. In Section 5 we then present recurrences that include generalizations of the algorithms of Levinson and Schur as special cases. Next, in Section 6, we briefly review some of the arguments that should allow one to prove the weak stability of these recurrences when combined with a suitable look-ahead strategy. In Section 7 the close relation of Padé forms to biorthogonal polynomials is exploited to deduce the inverse block LDU factorization of a Toeplitz matrix. When look-ahead occurs, this factorization requires the computation of "inner" polynomials in addition to the well-column-regular ones. These inner polynomials are seen to correspond to "underdetermined" Padé forms. Finally, in Section 8 we present a new simplified version of a superfast look-ahead Schur-type algorithm.

2. Preliminaries. In this paper, we will denote by $\mathbb{Z}$ the set of all integers, by $\mathbb{N}$ the set of all nonnegative integers, and by $\mathbb{N}^+$ the set of all positive integers. Moreover, $\|\cdot\|$ will always denote the 2-norm.

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Let $\mathcal{L}$ denote the set of formal Laurent series with complex coefficients,

$$h(\zeta) := \sum_{k=-\infty}^{\infty} \mu_k \zeta^k, \tag{2.1}$$

and consider the subsets

$$\begin{aligned} \mathcal{L}_{l:m} &:= \{f \in \mathcal{L}\,;\ \mu_k = 0 \text{ if } k < l \text{ or } k > m\}, \\ \mathcal{L}_l &:= \{h \in \mathcal{L}\,;\ \mu_k = 0 \text{ if } k < l\}, \\ \mathcal{L}_m^* &:= \{h \in \mathcal{L}\,;\ \mu_k = 0 \text{ if } k > m\}. \end{aligned}$$

Furthermore, denote by $\mathcal{P}_m (= \mathcal{L}_{0:m})$ the set of polynomials of degree at most m. Note that the quotient of $h \in \mathcal{L}_l$ and $q \in (\mathcal{P}_n \backslash \{0\})$ can be expanded according to rising powers of ζ, so that the result is in $\mathcal{L}_l$ if $q(0) \neq 0$. The Laurent series of this formal quotient is written as $L_+(h/q)$. For $h \in \mathcal{L}_m^*$ (or $h \in \mathcal{L}_l$), the largest (or smallest) index k with $\mu_k \neq 0$ is denoted by ∂h (or $\partial^* h$, respectively). Consequently, for a polynomial q, ∂q is the exact degree and $\partial^* q$, if positive, is the multiplicity of $\zeta = 0$ as a zero of q. In general, we call ∂h the degree and $\partial^* h$ the codegree of h. Hence, $\mathcal{L}_{l:m}$ is the set of Laurent polynomials of codegree at least l and degree at most m.

We write $h(\zeta) = O_+(\zeta^l)$ if $h(\zeta) \in \mathcal{L}_l$, and $h(\zeta) = O_-(\zeta^m)$ if $h(\zeta) \in \mathcal{L}_m^*$. If $h \in \mathcal{L}_0$ we set $h(0) := \mu_0$, and likewise, if $h \in \mathcal{L}_0^*$ we define $h(\infty) := \mu_0$. The formal projection of $h \in \mathcal{L}$ into $\mathcal{L}_{l:m}$ is denoted by

$$\Pi_{l:m} h(\zeta) := \sum_{k=l}^{m} \mu_k \zeta^k. \tag{2.2}$$

The (one-sided) Padé forms and Padé approximants of $h \in \mathcal{L}$ can be defined as follows; see [7, 36, 20].

Definition. Given a formal Laurent series $h \in \mathcal{L}$ and integers $(m, n) \in \mathbb{Z} \times \mathbb{N}$, any pair $(p, q) \in \mathcal{L}_m^* \times (\mathcal{P}_n \backslash \{0\})$ satisfying

$$h(\zeta)q(\zeta) - p(\zeta) = O_+(\zeta^{m+n+1}) \in \mathcal{L}_{m+n+1} \tag{2.3}$$

is a (*one-sided*) (m, n) *Padé form* of h. The series $e \in \mathcal{L}_0$ defined implicitly by

$$h(\zeta)q(\zeta) - p(\zeta) = \zeta^{m+n-1} e(\zeta) \tag{2.4}$$

is the *residual* of (p, q). The formal Laurent series

$$r_{m,n}(\zeta) := h(z) - L_+\left(\frac{h(\zeta)q(\zeta) - p(\zeta)}{q(\zeta)}\right) \tag{2.5}$$

is called the (*one-sided*) (m, n) *Padé approximant* of h.

Clearly Padé forms are never uniquely determined because p and q can be multiplied by a common nonzero scalar; for the situation of interest to us we will discuss normalization later. On the other hand, one can show that $r_{m,n}$ is uniquely determined. When h is just a formal power series and $m \geq 0$, the above definition can be seen to be equivalent with the classical one, where $r_{m,n} := p/q$ is a rational function of type (m, n); see, *e.g.*, Gragg [19] for a survey of classical results in Padé approximation.

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It is common to think of the Padé approximants of h as being listed in a table whose (m,n) entry is $r_{m,n}$. In the present situation this *Padé table* is defined in the half-plane $n \geq 0$. As in [19] we let the n-axis point to the right, and the m-axis to the bottom. A fundamental property of the Padé table is that equal entries always appear in square blocks. In the cases where the Padé approximant is equal to h or the zero function, these blocks are "infinite squares". This block structure property is derived by discussing the general solution of condition (2.3). The following result is fundamental; see [19, 7, 20].

THEOREM 2.1. *Given $h \in \mathcal{L}$, $m \in \mathbb{Z}$, and $n \in \mathbb{N}$, the general solution $(p,q) \in \mathcal{L}^*_m \times (\mathcal{P}_n \setminus \{0\})$ of* (2.3) *is*

$$(p(\zeta), q(\zeta)) = (\zeta^\sigma \breve{p}_{m,n}(\zeta)\, w(\zeta), \zeta^\sigma \breve{q}_{m,n}(\zeta)\, w(\zeta)), \tag{2.6}$$

where $\breve{p}_{m,n} \in \mathcal{L}^*_m$ and $\breve{q}_{m,n} \in \mathcal{P}_n$ with $\breve{q}_{m,n}(0) = 1$ are uniquely determined, and where

$$\sigma := \sigma_{m,n} := \max\{0, m+n+1 - \partial^*(h\breve{q}_{m,n} - \breve{p}_{m,n})\} \tag{2.7}$$

is a fixed integer satisfying

$$0 \leq \sigma \leq \delta := \delta_{m,n} := \min\{m - \partial\breve{p}_{m,n}, n - \partial\breve{q}_{m,n}\}, \tag{2.8}$$

and $w \in \mathcal{P}_{\delta-\sigma}$ is arbitrary.

By comparing in (2.3) the coefficients of $\zeta^{m+1}, \ldots, \zeta^{m+n}$, we readily obtain a homogeneous linear system with an $n \times (n+1)$ Toeplitz matrix for the coefficients $\rho_0, \rho_1, \ldots, \rho_n$ of q:

$$\begin{bmatrix} \mu_{m+1} & \mu_m & \cdots & \mu_{m-n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{m+n} & \mu_{m+n-1} & \cdots & \mu_m \end{bmatrix} \begin{bmatrix} \rho_0 \\ \rho_1 \\ \vdots \\ \rho_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{2.9}$$

As mentioned in the introduction, it is well known that the recursive solution of this system is linked to the computation of a finite sequence of Padé forms. In particular, the leading principal submatrices of the Toeplitz matrix correspond to the Padé approximants that lie in the mth row of the Padé table on the left of the (m,n) entry. The classical algorithms of Levinson (or Levinson-Durbin) [26, 16] and Schur (or Schur-Bareiss) [32, 4] can be understood to follow simultaneously the $(m-1)$th and the mth row of the table.

In the sequel we therefore consider two adjacent *row sequences* $\{(\hat{p}_n, \hat{q}_n)\}_{n=0}^\infty := \{(p_{m-1,n}, q_{m-1,n})\}$ and $\{(p_n, q_n)\}_{n=0}^\infty := \{(p_{m,n}, q_{m,n})\}$ of Padé forms, and the corresponding sequences $\{\hat{r}_n\}_{n=0}^\infty := \{r_{m-1,n}\}_{n=0}^\infty$ and $\{r_n\}_{n=0}^\infty := \{r_{m,n}\}_{n=0}^\infty$ of Padé approximants. The corresponding residuals are denoted by e_n and $\hat{e}_n$. They satisfy

$$\begin{bmatrix} -1 & h \end{bmatrix} \begin{bmatrix} \hat{p}_n & p_n \\ \hat{q}_n & q_n \end{bmatrix} = \zeta^{m+n} \begin{bmatrix} \hat{e}_n & \zeta e_n \end{bmatrix}. \tag{2.10}$$

The coefficients of the series $\hat{e}_n$, e_n, $\hat{p}_n$, p_n, and of the polynomials $\hat{q}_n$ and q_n are

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chosen as follows:[2]

$$
\begin{aligned}
\hat{e}_n(\zeta) \quad &=: \quad \sum_{k=n}^{\infty} \hat{\varepsilon}_{k,n} \zeta^{k-n}, & e_n(\zeta) \quad &=: \quad \sum_{k=n}^{\infty} \varepsilon_{k,n} \zeta^{k-n}, \\
\hat{p}_n(\zeta) \quad &=: \quad \sum_{k=0}^{\infty} \hat{\pi}_{k,n}\, \zeta^{m-1-k}, & p_n(\zeta) \quad &=: \quad \sum_{k=0}^{\infty} \pi_{k,n}\, \zeta^{m-k}, \\
\hat{q}_n(z) \quad &=: \quad \sum_{k=0}^{n} \hat{\rho}_{k,n}\, \zeta^{k}, & q_n(z) \quad &=: \quad \sum_{k=0}^{n} \rho_{k,n}\, \zeta^{k}.
\end{aligned}
\tag{2.11}
$$

If the $n \times n$ Toeplitz matrix

$$
\mathbf{T}_{m;n} := \begin{bmatrix} \mu_m & \cdots & \mu_{m-n+1} \\ \vdots & \ddots & \vdots \\ \mu_{m+n-1} & \cdots & \mu_m \end{bmatrix}
\tag{2.12}
$$

is nonsingular, it follows from (2.9) that we can normalize $\hat{q}_n$ by $\hat{\rho}_{n,n} := 1$ and q_n by $\rho_{0,n} := q_n(0) := 1$; *i.e.*, $\hat{q}_n$ can be chosen monic, q_n comonic. With these normalizations (2.9) yields the *Yule-Walker equations*

$$
\mathbf{T}_{m;n} \begin{bmatrix} \hat{\rho}_{0,n} \\ \vdots \\ \hat{\rho}_{n-1,n} \end{bmatrix} = - \begin{bmatrix} \mu_{m-n} \\ \vdots \\ \mu_{m-1} \end{bmatrix}, \quad \mathbf{T}_{m;n} \begin{bmatrix} \rho_{1,n} \\ \vdots \\ \rho_{n,n} \end{bmatrix} = - \begin{bmatrix} \mu_{m+1} \\ \vdots \\ \mu_{m+n} \end{bmatrix}.
\tag{2.13}
$$

One can conclude from (2.3) and (2.4) that also the following two linear systems hold:

$$
\mathbf{T}_{m;n+1} \begin{bmatrix} \hat{\rho}_{0,n} \\ \vdots \\ \hat{\rho}_{n-1,n} \\ \hat{\rho}_{n,n} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \hat{\varepsilon}_{n,n} \end{bmatrix}, \quad \mathbf{T}_{m;n+1} \begin{bmatrix} \rho_{0,n} \\ \rho_{1,n} \\ \vdots \\ \rho_{n,n} \end{bmatrix} = \begin{bmatrix} \pi_{0,n} \\ 0 \\ \vdots \\ 0 \end{bmatrix}.
\tag{2.14}
$$

Each of them represents just $n+1$ rows of a doubly infinite linear Toeplitz systems whose right-hand side contains the coefficients of $\hat{p}_n$ (or p_n, respectively) in its "upper half" and those of $\hat{e}_n$ (or e_n) in its "lower half", the two sets being separated by the n zeros that appear in (2.14).

3. Column-regular Padé forms. The algorithms discussed in this paper make essential use of column-regular and well-column-regular Padé forms. These notions have been introduced in [20].

Definition. We call the Padé form (p_n, q_n) and the approximant $r_n := p_n/q_n$ *column-regular* if

$$
\hat{p}_n q_n - p_n \hat{q}_n \neq 0 \ \in \mathcal{L}.
\tag{3.1}
$$

We also say that $(\hat{p}_n, \hat{q}_n)$ and (p_n, q_n) is a *column-regular pair* (of Padé forms), and that n is a *column-regular index*.

From (2.5) it is readily seen that r_n is column-regular if and only if $r_n \neq \hat{r}_n$, *i.e.*, if in the Padé table, r_n is not in the same block as the entry $\hat{r}_n$ above it, see

[2] Note that the notation used in this paper differs partially from the one chosen in [22], where $\varepsilon_{n+k,n}$ was $\pi_{k,n}$, $\pi_{k,n}$ was $\varepsilon_{n+k,n}$, and $\rho_{k,n}$ was $\rho_{n-k,n}$.

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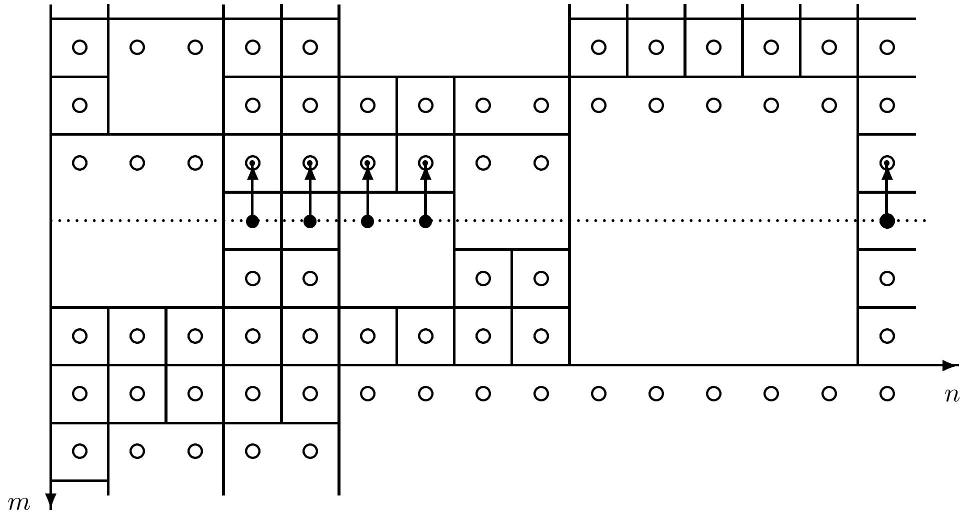

FIG. 3.1. *Column-regular entries marked by ∘ in the extended Padé table. In one row they are marked by • and their upper neighbors by a dot.*

Fig. 1. In other words, r_n is column-regular if and only if it lies in the first row of its block. From Theorem 2.1 one can further conclude that column-regular Padé forms are uniquely determined up to scaling, since, for column-regularity, $\delta_{m,n} = \sigma_{m,n} = 0$ and $\delta_{m-1,n} = \sigma_{m-1,n}$.

Further characterizations of column-regularity are summarized in the following Lemma.

LEMMA 3.1. *The following statements are equivalent when $n \geq 0$:*

(i) (p_n, q_n) *is column-regular, i.e.,* (3.1) *holds;*

(ii) $r_n \neq \hat{r}_n$*;*

(iii) $\partial p_n = m$ *and* $\partial \hat{q}_n = n$*; i.e.,* $\pi_{0,n} \neq 0$ *and* $\hat{\rho}_{n,n} \neq 0$*;*

(iv) $\hat{e}_n(0) \neq 0$ *and* $q_n(0) \neq 0$*; i.e.,* $\hat{\varepsilon}_{n,n} \neq 0$ *and* $\rho_{0,n} \neq 0$*;*

(v) *the Toeplitz matrices* $\mathbf{T}_{m;n}$ *and* $\mathbf{T}_{m;n+1}$ *are nonsingular;*

(vi) *the Yule-Walker equations* (2.13) *have a unique pair of solutions, and the corresponding residual* $\hat{e}_n$ *and numerator* p_n *satisfy* $\hat{e}_n(0) \neq 0$ *and* $\partial p_n = m$*;*

(vii) *the Yule-Walker equations* (2.13) *have a pair of solutions whose corresponding residual* $\hat{e}_n$ *and numerator* p_n *satisfy* $\hat{e}_n(0) \neq 0$ *and* $\partial p_n = m$*;*

(viii) q_n *and* $\hat{q}_n$ *are relatively prime, and* $\partial p_n = m$ *if* q_n *is a (nonzero) constant.*

(*If* $n = 0$*, the empty matrix* $\mathbf{T}_{m,n}$ *is considered to be nonsingular, and the Yule-Walker equations are considered to have a unique vacuous solution.*)

Note that (iii)–(viii) translate immediately into the conditions (iii), (iv), (ii), (i), (v), and (vii) of Lemma 4.1 in [22]. As mentioned before, the notation chosen there partially differs from the one used here, however, and $m = 0$ was assumed.

Proof. The equivalence of (i) and (ii) follows from (2.5): the two series $L_+((hq-p)/q)$ and $L_+((h\hat{q}-\hat{p})/q)$ are the same if and only if (3.1) holds. The equivalence of (ii) with (iii), (iv), (v), and (vi) was shown in [20] (under slightly different assumptions, to which the case treated here could be reduced, however). The main tools were Theorem 2.1 and the block structure theorem mentioned before that follows from it. Finally, (vi) clearly implies (vii). Hence, it remains to show that

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(vii) implies, say, (ii) and that (viii) is equivalent with, say, (i). The proof of this equivalence will also furnish, for free, another simple proof of the equivalence of (i), (iii), and (iv).

Assume that (vii) holds. Then there exists an $(m-1, n)$ Padé form $(\hat{p}_n, \hat{q}_n)$ with monic $\hat{q}_n$ and $\hat{\varepsilon}_{n,n} \neq 0$. From Theorem 2.1 it follows that this means that $\hat{r}_n$ lies both on or below the diagonal and on or below the antidiagonal of its block. Additionally there exists an (m, n) Padé form (p_n, q_n) with $q_n(0) = 1$ and $\partial p_n = m$. Here one can conclude from Theorem 2.1 that r_n must lie both on or above the diagonal and on or above the antidiagonal of its block. Since $\hat{r}_n$ is the upper neighbor of r_n, the only way to fulfill these conditions is that $\hat{r}_n$ and r_n lie in different blocks; hence, (ii) holds.

In [20], Lemma 2.5, we pointed out that (2.3) implies readily that

$$\hat{p}_n(\zeta) q_n(\zeta) - p_n(\zeta)\hat{q}_n(\zeta) = \hat{\Delta}_n \zeta^{m+n}\,; \tag{3.2}$$

i.e., this Laurent series has at most one nonzero coefficient $\hat{\Delta}_n$. In addition, from (3.2) and (2.3), it is easily verified that

$$\hat{\Delta}_n = \pi_{0,n}\hat{\rho}_{n,n} = \hat{\varepsilon}_{n,n}\rho_{0,n} \;\; [= \hat{e}_n(0) q_n(0)]. \tag{3.3}$$

Hence, (p_n, q_n) is column-regular if and only if $\hat{\Delta}_n \neq 0$. If q_n and $\hat{q}_n$ are not relatively prime, they have a common polynomial factor, which must also be a factor of the right-hand side in (3.2), unless the right-hand side is zero. However, $\hat{\Delta}_n z^{m+n}$ has only monomials as factors. Thus, $\hat{\Delta}_n = 0$ or $\hat{q}_n(0) = q_n(0) = 0$. In both cases, q_n is not column-regular. [Consequently, $\hat{q}_n(0) = q_n(0) = 0$ implies $\hat{\Delta}_n = 0$.] Moreover, if q_n is a nonzero constant and $\partial p_n < m$, then (p_n, q_n) is also an $(m-1, n)$ Padé form, hence not column-regular.

Conversely, if q_n is not column-regular, then, by (ii), $r_n = \hat{r}_n$. If $h \in \mathcal{L}_L$ for some L (as, *e.g.*, in the classical situation where $L = 0$), then r_n and $\hat{r}_n$ are rational functions and must have a common reduced form, whose denominator $\breve{q}_{m,n}$ is a common factor of q_n and $\hat{q}_n$. The general case $h \in \mathcal{L}$ can be reduced to this one since q_n and $\hat{q}_n$ only depend on finitely many coefficients of h. Consequently, q_n and $\hat{q}_n$ cannot be mutually prime unless $\breve{q}_{m,n}(\zeta) \equiv 1$. In the latter case, it follows that $\hat{r}_n = r_n \in \mathcal{L}^*_{m-1}$; hence, $q_n(\zeta) \equiv 1$ implies that $\partial p_n < m$ if q_n is not column-regular.

Note that (3.2) and (3.3) imply that each of (i), (iii), and (iv) is equivalent to $\hat{\Delta}_n \neq 0$. □

In view of statements (iii)-(v) of Lemma 3.1, column-regular pairs of Padé forms can be normalized by

$$\hat{\rho}_{n,n} = 1, \quad \rho_{0,n} = 1, \tag{3.4}$$

as was assumed for the Yule-Walker equations (2.13). Then, by (3.3),

$$\pi_{0,n} = \hat{\varepsilon}_{n,n}. \tag{3.5}$$

Formula (2.10) defines the residuals $\hat{e}_n$ and e_n as functions of the data h and the pair $(\hat{p}_n, \hat{q}_n)$, (p_n, q_n) of Padé forms. It is an important fact that if this pair is column-regular, then this pair and its two residuals allow us to retrieve the data. This shows that all the information on the problem is stored in any column-regular pair and the corresponding two residuals. In fact, (2.10) has the following converse: if (p_n, q_n) is column-regular, then

$$\begin{bmatrix} -1 & h \end{bmatrix} = \frac{1}{\hat{\Delta}_n}\begin{bmatrix} \hat{e}_n & \zeta e_n \end{bmatrix} \begin{bmatrix} q_n & -p_n \\ -\hat{q}_n & \hat{p}_n \end{bmatrix}, \tag{3.6}$$

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where $\hat{\Delta}_n$ is given by (3.3). For the proof one postmultiplies (2.10) by the 2×2 matrix from (3.6) and inserts (3.2).

Clearly, column-regularity cannot guarantee that a corresponding Padé form is numerically well determined, *i.e.*, depends in a well-conditioned way on the data, the given coefficientes μ_k. In fact, the Toeplitz matrix appearing in the Yule-Walker equations (2.13) for the coefficients of the polynomial q of a column-regular Padé form (p, q) could be arbitrarily ill conditioned. In this case we will also call the Padé form (p, q) ill conditioned. Recursive processes that make at an intermediate stage use of such ill-conditioned Padé forms cannot be stable either. The basic philosophy of look-ahead algorithms consist in avoiding such ill-conditioned intermediate results. Here, in particular, we will later require that Padé forms are not only column-regular, but also well-conditioned functions of the data, and we will call such Padé forms well-column-regular. We will return to this issue in Section 6.

4. Column-regular two-point Padé forms. As in [20] our look-ahead recurrences will make use of certain two-point Padé forms. Therefore, let us recall from [20] the definition of an $[l;k]$ two-point Padé form $(u_k, v_k) \in \mathcal{P}_{k-1}\times\mathcal{P}_k$ of a quadruple of formal power series $(f^-, g^-; f^+, g^+)$ given by

$$f^-(\zeta) =: \sum_{k=1}^{\infty} \phi_k^- \zeta^{-k}, \qquad f^+(\zeta) =: \sum_{k=0}^{\infty} \phi_k^+ \zeta^{k}, \tag{4.1}$$

$$g^-(\zeta) =: \sum_{k=0}^{\infty} \gamma_k^- \zeta^{-k}, \qquad g^+(\zeta) =: \sum_{k=0}^{\infty} \gamma_k^+ \zeta^{k}. \tag{4.2}$$

We assume that these formal power series fulfill at least one of the following two pairs of conditions

$$\phi_1^- \neq 0 \quad \text{and} \quad \gamma_0^+ \neq 0, \tag{4.3}$$

$$\gamma_0^- \neq 0 \quad \text{and} \quad \gamma_0^+ \neq 0. \tag{4.4}$$

Definition. Given a pair $[l;k]$ of integers satisfying $|l| < k$ or $|l| = k > 0$, a pair $(u, v) \in \mathcal{P}_{k-1}\times\mathcal{P}_k$ is an $[l;k]$ *two-point Padé form* of $(f^-, g^-; f^+, g^+)$ if

$$\begin{aligned} g^-(\zeta)u(\zeta) + f^-(\zeta)v(\zeta) &= O_-(\zeta^{l-1}) \in \mathcal{L}_{l-1}^*, \\ g^+(\zeta)u(\zeta) + f^+(\zeta)v(\zeta) &= O_+(\zeta^{k+l}) \in \mathcal{L}_{k+l}. \end{aligned} \tag{4.5}$$

The rational function $u(\zeta)/v(\zeta)$ is said to be the $[l;k]$ *two-point Padé approximant* of $(f^-, g^-; f^+, g^+)$. The *residual* of (u, v) consists of two series $(e^-; e^+) \in \mathcal{L}_0^\star \times \mathcal{L}_0$ defined by

$$\begin{aligned} g^-(\zeta)u(\zeta) + f^-(\zeta)v(\zeta) &= \zeta^{l-1}e^-(\zeta), \\ g^+(\zeta)u(\zeta) + f^+(\zeta)v(\zeta) &= \zeta^{k+l}e^+(\zeta). \end{aligned} \tag{4.6}$$

Again, it can be shown that the $[l;k]$ two-point Padé approximant is uniquely determined. These two-point Padé approximants can be thought of being gathered in a double-entry table, the two-point Padé table, where, however, they only fill the sector $|l| \le k$ of the half-plane $k > 0$. If $|l| = k > 0$, either the first or the second condition of (4.5) is vacuous, and the two-point Padé approximant reduces essentially to an ordinary Padé approximant. By generalizing the definition, so that it includes additional suitably chosen Padé approximants, the table can be extended to fill the

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whole half-plane $k \geq 0$. It is then called M-table; see [27, 13]. A block structure theorem analogous to the one for the ordinary Padé table holds; see [13, 20].

In the following l will be fixed, and $k \geq \max\{|l|, |l-1|\}$, so that $-k+1 \leq l \leq k$. We denote the $[l;k]$ two-point Padé form by (u_k, v_k) and the $[l-1;k]$ two-point Padé form by $(\hat{u}_k, \hat{v}_k)$. The corresponding residuals are called (e_k^-, e_k^+) and $(\hat{e}_k^-, \hat{e}_k^+)$. In analogy to (2.10), they satisfy

$$\begin{bmatrix} g^- & f^- \\ g^+ & f^+ \end{bmatrix} \begin{bmatrix} \hat{u}_k & u_k \\ \hat{v}_k & v_k \end{bmatrix} = \begin{bmatrix} \zeta^{l-2} & 0 \\ 0 & \zeta^{k+l-1} \end{bmatrix} \begin{bmatrix} \hat{e}_k^- & \zeta e_k^- \\ \hat{e}_k^+ & \zeta e_k^+ \end{bmatrix}. \tag{4.7}$$

The coefficients of these two-point Padé forms are chosen as follows:[3]

$$\hat{u}_k(\zeta) =: \sum_{j=0}^{k-1} \hat{\alpha}_{j,k}\zeta^j, \qquad \hat{v}_k(\zeta) =: \sum_{j=0}^{k} \hat{\beta}_{j,k}\zeta^j, \tag{4.8}$$

$$u_k(\zeta) =: \sum_{j=0}^{k-1} \alpha_{j,k}\zeta^j, \qquad v_k(\zeta) =: \sum_{j=0}^{k} \beta_{j,k}\zeta^j. \tag{4.9}$$

Thus we are considering again two adjacent rows of the table. Later we will set $l := 0$, and we will see that in our situation $\hat{\beta}_{k,k} = \beta_{k,k} = 0$, *i.e.*, the polynomials $\hat{v}_k$ and v_k have at most degree $k-1$ also.

We first adapt the notion of column regularity to the two-point Padé table.

DEFINITION. We call the two-point Padé form (u_k, v_k) and the approximant u_k/v_k *column-regular* if

$$\hat{u}_k v_k - u_k \hat{v}_k \neq 0 \;\in \mathcal{P}, \quad i.e., \quad \frac{u_k}{v_k} \neq \frac{\hat{u}_k}{\hat{v}_k}. \tag{4.10}$$

We also say that $(\hat{u}_k, \hat{v}_k)$, (u_k, v_k) are a *column-regular pair* (of two-point Padé forms).

The following result is an analogue of (3.2) and (3.3).

LEMMA 4.1. *Let (u_k, v_k) be an $[l;k]$ two-point Padé form, and $(\hat{u}_k, \hat{v}_k)$ be an $[l-1;k]$ two-point Padé form of a quadruple $(f^-, g^-; f^+, g^+)$ that fulfills* (4.3) *or* (4.4). *Then,*

$$\hat{u}_k v_k - u_k \hat{v}_k = \hat{\Delta}_{l;k}\zeta^{k+l-1}, \tag{4.11}$$

where

$$\hat{\Delta}_{l;k} = \hat{e}_k^+(0)\beta_{0,k}/\gamma_0^+ = \begin{cases} e_k^-(\infty)\hat{\alpha}_{k-1,k}/\phi_1^- & \text{if } \phi_1^- \neq 0, \\ -e_k^-(\infty)\hat{\beta}_{k,k}/\gamma_0^- & \text{if } \gamma_0^- \neq 0. \end{cases} \tag{4.12}$$

Proof. From (4.7) we have

$$g^-\hat{u}_k + f^-\hat{v}_k = \zeta^{l-2}\hat{e}_k^- = O_-(\zeta^{l-2}), \qquad g^+\hat{u}_k + f^+\hat{v}_k = \zeta^{k+l-1}\hat{e}_k^+ = O_+(\zeta^{k+l-1}), \tag{4.13}$$

$$g^-u_k + f^-v_k = \zeta^{l-1}e_k^- = O_-(\zeta^{l-1}), \qquad g^+u_k + f^+v_k = \zeta^{k+l}e_k^+ = O_+(\zeta^{k+l}). \tag{4.14}$$

Multiplying the second equation in (4.13) by v_k and the second equation in (4.14) by $\hat{v}_k$, and subtracting the two results yields

$$g^+(\hat{u}_k v_k - u_k \hat{v}_k) = \zeta^{k+l-1}(\hat{e}_k^+ v_k - \zeta e_k^+ \hat{v}_k).$$

[3] In [22], $\alpha_{j,k}$ was β_j, $\beta_{j,k}$ was α_{k-j-1}, and $\hat{\beta}_{j,k}$ was $\hat{\beta}_{k-j-1}$.

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By assumptions (4.3) and (4.4), we have $\gamma_0^+ = g^+(0) \neq 0$, and therefore

$$\hat{u}_k v_k - u_k \hat{v}_k = \zeta^{k+l-1} \hat{e}_k^+(0) \beta_{0,k}/\gamma_0^+ + O_+(\zeta^{k+l}).$$

Analogously, from the first equations in (4.13) and (4.14) we obtain

$$g^-(\hat{u}_k v_k - u_k \hat{v}_k) = \zeta^{l-2}(\hat{e}_k^- v_k - \zeta e_k^- \hat{v}_k), \quad f^-(\hat{u}_k v_k - u_k \hat{v}_k) = -\zeta^{l-2}(\hat{e}_k^- u_k - \zeta e_k^- \hat{u}_k).$$

Hence,

$$\hat{u}_k v_k - u_k \hat{v}_k = \begin{cases} \zeta^{k+l-1} e_k^-(\infty) \hat{\alpha}_{k-1,k}/\phi_1^- + O_-(\zeta^{k+l-2}) & \text{if } \phi_1^- \neq 0, \\ -\zeta^{k+l-1} e_k^-(\infty) \hat{\beta}_{k,k}/\gamma_0^- + O_-(\zeta^{k+l-2}) & \text{if } \gamma_0^- \neq 0. \end{cases}$$

This completes the proof. ◻

Lemma 4.1 leads easily to the following partial analogue of Lemma 3.1.

LEMMA 4.2. *Let the assumptions of Lemma* 4.1 *be satisfied. Then, the following statements are equivalent when $k > 0$ and $-k+1 \leq l \leq k$:*

(i) (u_k, v_k) *is column-regular, i.e.,* (4.10) *holds;*
(ii) $\hat{e}_k^+(0) \neq 0$ *and* $\beta_{0,k} \neq 0$.
(iii) $e_k^-(\infty) \neq 0$ *and* $\hat{\alpha}_{k-1,k} \neq 0$ *if* $\phi_1^- \neq 0$, *and* $e_k^-(\infty) \neq 0$ *and* $\hat{\beta}_{k,k} \neq 0$ *if* $\gamma_0^- \neq 0$.

Proof. (i) is equivalent to $\hat{\Delta}_{k;l} \neq 0$ in (4.11). Hence, the two other equivalences follow readily from the different expressions for $\hat{\Delta}_{k;l}$ in (4.12). ◻

In view of statements (iii) and (iv) of Lemma 3.1, column-regular pairs of two-point Padé forms can be normalized by

$$\begin{array}{lllllll} \hat{\alpha}_{k-1,k} & = & 1, & \beta_{0,k} & = & 1, & \text{if } \phi_1^- \neq 0, \\ \hat{\beta}_{k,k} & = & 1, & \beta_{0,k} & = & 1, & \text{if } \gamma_0^- \neq 0. \end{array} \tag{4.15}$$

We will make use of this normalization shortly.

In analogy to (3.6) one can express also the data $(f^-, g^-; f^+, g^+)$ of the two-point Padé problem in terms of any column-regular pair and its residuals. Again we just have to postmultiply (4.7) by the inverse of the second 2×2 matrix and to make use of (4.11):

$$\begin{bmatrix} g^- & f^- \\ g^+ & f^+ \end{bmatrix} = \frac{1}{\hat{\Delta}_{l;k}} \begin{bmatrix} \zeta^{1-k} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{e}_k^- & \zeta e_k^- \\ \hat{e}_k^+ & \zeta e_k^+ \end{bmatrix} \begin{bmatrix} v_k & -u_k \\ -\hat{v}_k & \hat{u}_k \end{bmatrix}. \tag{4.16}$$

Let us next consider the linear systems which have to be solved for computing a normalized regular pair of two-point Padé forms. For the look-ahead Levinson and Schur recurrences, we will need the cases $l = 0$ and $l = -1$ only. Moreover, the data will be seen to always fulfill $\gamma_0^- = 0$ and (4.3), which implies that $\beta_{k,k} = \hat{\beta}_{k,k} = 0$. The conditions (4.13) and (4.14) translate into two homogeneous systems of $2k-1$ linear equations for the $2k$ remaining unknown coefficients of $(\hat{u}_k, \hat{v}_k) \in \mathcal{P}_{k-1} \times \zeta\mathcal{P}_{k-1}$ and $(u_k, v_k) \in \mathcal{P}_{k-1} \times \zeta\mathcal{P}_{k-1}$, respectively; see Eq. (3.20) in [20]. Due to the normalization (4.15) we can move one column of the coefficient matrix to the right-hand side. Moreover, since $\gamma_0^- = 0$, each of the two systems contains one equation that depends on just one unknown and, therefore, can be used to eliminate that unknown. Making use of $\beta_{0,k} = 1$ and $\gamma_0^- = 0$ in this way, we obtain from (4.14) with $l = 0$, the two equations

$$\alpha_{0,k} = -\phi_0^+/\gamma_0^+, \quad \beta_{k,k} = 0 \tag{4.17}$$

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and the $2(k-1) \times 2(k-1)$ system

$$\mathbf{S}_{k-1} \left[\begin{array}{c} \alpha_{1,k} \\ \vdots \\ \alpha_{k-1,k} \\ \hline \beta_{1,k} \\ \vdots \\ \beta_{k-1,k} \end{array} \right] = - \left[\begin{array}{c} 0 \\ \vdots \\ 0 \\ \hline \phi_1^+ \\ \vdots \\ \phi_{k-1}^+ \end{array} \right] - \left[\begin{array}{c} 0 \\ \vdots \\ 0 \\ \hline \gamma_1^+ \\ \vdots \\ \gamma_{k-1}^+ \end{array} \right] \alpha_{0,k}, \tag{4.18}$$

where

$$\mathbf{S}_{k-1} = \left[\begin{array}{ccc|ccc} \gamma_1^- & \cdots & \gamma_{k-1}^- & \phi_1^- & \cdots & \phi_{k-1}^- \\ & \ddots & \vdots & & \ddots & \vdots \\ & & \gamma_1^- & & & \phi_1^- \\ \hline \gamma_0^+ & & & \phi_0^+ & & \\ \vdots & \ddots & & \vdots & \ddots & \\ \gamma_{k-2}^+ & \cdots & \gamma_0^+ & \phi_{k-2}^+ & \cdots & \phi_0^+ \end{array} \right]. \tag{4.19}$$

From (4.13) with $l = -1$ we obtain likewise, taking $\hat{\alpha}_{k-1,k} = 1$ and $\gamma_0^- = 0$ into account, the two equations

$$\hat{\beta}_{0,k} = -\gamma_1^- / \phi_1^-, \quad \hat{\beta}_{k,k} = 0 \tag{4.20}$$

and the linear system

$$\mathbf{S}_{k-1} \left[\begin{array}{c} \hat{\alpha}_{0,k} \\ \vdots \\ \hat{\alpha}_{k-2,k} \\ \hline \hat{\beta}_{1,k} \\ \vdots \\ \hat{\beta}_{k-1,k} \end{array} \right] = - \left[\begin{array}{c} \gamma_k^- \\ \vdots \\ \gamma_1^- \\ \hline 0 \\ \vdots \\ 0 \end{array} \right] - \left[\begin{array}{c} \phi_k^- \\ \vdots \\ \phi_1^- \\ \hline 0 \\ \vdots \\ 0 \end{array} \right] \hat{\beta}_{0,k} \tag{4.21}$$

with the same coefficient matrix. For $k = 1$, the linear systems (4.18) and (4.21) are empty; the coefficients are fully determined by (4.17) and (4.20).

Clearly, every pair of solutions of (4.17)–(4.21) yields a pair of normalized two-point Padé forms. From Lemma 4.2 (ii) and (iii) we know that such a pair is column-regular if and only if $\hat{e}_k^+(0) \neq 0$ and $e_k^-(\infty) \neq 0$. We also know that these two quantities always vanish simultaneously. By definition they are given by

$$\begin{aligned} \hat{e}_k^+(0) &= \textstyle\sum_{j=0}^k \left(\gamma_j^+ \hat{\alpha}_{k-j-1,k} + \phi_j^+ \hat{\beta}_{k-j-1,k} \right), \\ e_k^-(\infty) &= \textstyle\sum_{j=0}^k \left(\gamma_{j+1}^- \alpha_{j,k} + \phi_{j+1}^- \beta_{j,k} \right). \end{aligned} \tag{4.22}$$

The first formula is the inhomogeneous equation that extends (4.21) at the bottom, the other is the one that extends (4.18) at the top. Bringing the right-hand sides of (4.18) and (4.21) back on the left-hand side, one obtains two inhomogeneous systems with matrix $\mathbf{S}_k$ and right-hand sides $\mathbf{e}_1 e_k^-(\infty)$ and $\mathbf{e}_{2k} \hat{e}_k^+(0)$, respectively. From Cramer's rule one can conclude (see [22], Eq. (5.22)) that

$$\hat{\alpha}_{k-1,k} \det \mathbf{S}_k = \phi_1^- \, \hat{e}_k^+(0) \det \mathbf{S}_{k-1}, \quad \beta_{0,k} \det \mathbf{S}_k = \gamma_0^+ \, e_k^-(\infty) \det \mathbf{S}_{k-1}. \tag{4.23}$$

By continuity these relations remain true as $\hat{e}_k^+(0) \to 0$, $e_k^-(\infty) \to 0$ or $\det \mathbf{S}_{k-1} \to 0$. Hence, if the pair is normalized (*i.e.*, $\hat{\alpha}_{k-1,k} = \beta_{0,k} = 1$) and $\det \mathbf{S}_{k-1} \neq 0$, each of the two conditions $\hat{e}_k^+(0) \neq 0$ and $e_k^-(\infty) \neq 0$ is equivalent to $\det \mathbf{S}_k \neq 0$. Moreover,

$$\phi_1^- \,\hat{e}_k^+(0) = \gamma_0^+ \,e_k^-(\infty). \tag{4.24}$$

This relation also follows from (4.12). On the other hand, if $\det \mathbf{S}_k \neq 0$, then $\det \mathbf{S}_{k-1} = 0$ implies that $\hat{\alpha}_{k-1,k} = \beta_{0,k} = 0$.

The Eqs. (4.17)–(4.21) are analogues of the Yule-Walker equations for the two-point Padé problem. They allow us to formulate analogues of the statements (v)–(vii) of Lemma 3.1. We also add the analogue of (viii), which follows from Lemma 4.1.

LEMMA 4.3. *Let the assumptions of Lemma* 4.1 *be satisfied, and suppose that the case $\gamma_0^- = 0$, $\gamma_0^+ \neq 0$, $\phi_1^- \neq 0$ is in effect. Then, the following statements are equivalent when $k > 0$ and $-k+1 \leq l \leq k$:*

(i) (u_k, v_k) *is column-regular, i.e.,* (4.10) *holds;*
(ii) *the matrices $\mathbf{S}_{k-1}$ and $\mathbf{S}_k$ are nonsingular;*
(iii) *the equations* (4.17)–(4.21) *have a unique pair of solutions, and the corresponding residuals $(e_k^-; e_k^+)$ and $(\hat{e}_k^-; \hat{e}_k^+)$ satisfy $e_k^-(\infty) \neq 0$ and $\hat{e}_k^+(0) \neq 0$;*
(iv) *the equations* (4.17)–(4.21) *have a pair of solutions whose corresponding residuals $(e_k^-; e_k^+)$ and $(\hat{e}_k^-; \hat{e}_k^+)$ satisfy $e_k^-(\infty) \neq 0$ and $\hat{e}_k^+(0) \neq 0$;*
(v) *v_n and $\hat{v}_n$ are relatively prime, and $\partial(g^- u_n + f^- v_n) = l-1$ if v_n is a (nonzero) constant.*

(*If $k = 1$, the empty matrix $\mathbf{S}_{k-1}$ is considered to be nonsingular, and equations* (4.18) *and* (4.21) *are considered to have a unique vacuous solution.*)

Proof. Assume $(\hat{u}_n, \hat{v}_n)$, (u_n, v_n) is a normalized column-regular pair. Note that with (u_n, v_n) any other $[l;k]$ two-point Padé form is also column-regular, since the quotient u/v is independent of the chosen two-point Padé form. Hence, by Lemma 4.2 (iii), the linear system with matrix $\mathbf{S}_k$ and right-hand side $\mathbf{e}_1 e_k^-(\infty)$ cannot have a nontrivial solution with $e_k^-(\infty) = 0$ or $\hat{\alpha}_{k-1,k} = 0$. Consequently, $\mathbf{S}_k$ is nonsingular, and in view of (4.23), $\mathbf{S}_{k-1}$ also is nonsingular; *i.e.*, (ii) holds. From the nonsingularity of $\mathbf{S}_{k-1}$ it follows that (4.17)–(4.21) have a unique pair of solutions. By (4.23) it follows further that $\det \mathbf{S}_k \neq 0$ implies $e_k^-(\infty) \neq 0$ and $\hat{e}_k^+(0) \neq 0$, as we have just seen. This completes the verification of (ii) $\Longrightarrow$ (iii). The implication (iii) $\Longrightarrow$ (iv) is trivial; and by Lemma 4.2, (iv) clearly implies that the corresponding two-point Padé form (u_n, v_n) is column-regular; hence, we are back at (i).

The proof of equivalence for (i) and (v) is basically the same as for the equivalence of statements (i) and (viii) of Lemma 3.1. The only difference is that, now, when v_n is a constant and (u_n, v_n) is an $[l;k]$ two-point Padé form, then the latter is not an $[l-1;k]$ two-point Padé form if and only if $e_k^-(\infty) \neq 0$, *i.e.*, $\partial(g^- u_n + f^- v_n) = l-1$. □

5. Look-ahead Levinson- and Schur-type recurrences. After these preliminaries we can formulate a theorem about general recurrence relations for the Padé table. As a special case it contains recurrences that follow two adjacent rows of the Padé table, as indicated in Fig. 1. They yield generalizations of both the algorithms of Levinson and Schur to nonnormal tables. Moreover, unlike some of the older algorithms that can only handle exact breakdowns, these recurrences are general enough to skip over near-breakdowns. Other algorithms that can handle near-breakdowns, but use different recurrences, were given in [11, 10, 12, 17, 20, 23].

THEOREM 5.1. *Let (p_n, q_n) be a column-regular (m,n) Padé form of $h \in \mathcal{L}$ with residual e_n, and let $(\hat{p}_n, \hat{q}_n)$ and $\hat{e}_n$ be an $(m-1,n)$ Padé form and its residual.*

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(i) If $|l| < k$ or $|l| = k > 0$, and if $(u_k^{(n)}, v_k^{(n)})$ is an $[l;k]$ two-point Padé form with residual (e_k^-, e_k^+) of

$$(f^-, g^-; f^+, g^+) := (\zeta^{-m-1} p_n, \zeta^{-m} \hat{p}_n; e_n, \hat{e}_n), \tag{5.1}$$

then $\partial v_k \le k-1$ holds, and the recurrence formula

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^{k+l} e_{n+k} \end{bmatrix} := \begin{bmatrix} \hat{p}_n & p_n \\ \hat{q}_n & q_n \\ \zeta^{-1}\hat{e}_n & e_n \end{bmatrix} \begin{bmatrix} \zeta u_k^{(n)} \\ v_k^{(n)} \end{bmatrix} \tag{5.2}$$

yields an $(m+l, n+k)$ Padé form (p_{n+k}, q_{n+k}) of h and its residual e_{n+k}, which is equal to e_k^+, while e_k^- is equal to $\zeta^{-m-l} p_{n+k}$.

(ii) If, moreover, $-k+1 \le l \le k$ and $(\hat{u}_k^{(n)}, \hat{v}_k^{(n)})$ is an $[l-1;k]$ two-point Padé form of (5.1) with residual $(\hat{e}_k^{(n)-}; \hat{e}_k^{(n)+})$, then $\partial \hat{v}_k^{(n)} \le k-1$ holds, and the recurrence formula

$$\begin{bmatrix} \hat{p}_{n+k} & p_{n+k} \\ \hat{q}_{n+k} & q_{n+k} \\ \zeta^{k+l-1}\hat{e}_{n+k} & \zeta^{k+l} e_{n+k} \end{bmatrix} := \begin{bmatrix} \hat{p}_n & p_n \\ \hat{q}_n & q_n \\ \zeta^{-1}\hat{e}_n & e_n \end{bmatrix} \begin{bmatrix} \zeta \hat{u}_k^{(n)} & \zeta u_k^{(n)} \\ \hat{v}_k^{(n)} & v_k^{(n)} \end{bmatrix} \tag{5.3}$$

yields in addition to the $(m+l, n+k)$ Padé form (p_{n+k}, q_{n+k}) and its residual e_{n+k} also an $(m+l-1, n+k)$ Padé form $(\hat{p}_{n+k}, \hat{q}_{n+k})$ of h and the corresponding residual $\hat{e}_{n+k}$, which is equal to $\hat{e}_k^{(n)+}$, while $\hat{e}_k^{(n)-}$ is equal to $\zeta^{-m-l+1}\hat{p}_{n+k}$. The new Padé form (p_{n+k}, q_{n+k}) is column-regular if and only if the two-point Padé form $(u_k^{(n)}, v_k^{(n)})$ is column-regular.

When the two-point Padé form $(u_k^{(n)}, v_k^{(n)})$ is column-regular, we say that $(n;k)$ is a *column-regular* index pair.

Proof. For simplicity we delete the upper index ${}^{(n)}$ in the proof.

(i) Consider (5.2) as the definition of its left-hand side. First, since $(u_k, v_k) \in \mathcal{P}_{k-1} \times \mathcal{P}_k$ and $\hat{q}_n, q_n \in \mathcal{P}_n$, it follows that $q_{n+k} \in \mathcal{P}_{n+k}$. Second, we note that $\partial p_n = m$ by Lemma 3.1(iii), and $\hat{e}_n(0) \ne 0$ by Lemma 3.1(iv). Hence, the data (5.1) satisfy (4.3). By definition of (u_k, v_k) as an $[l;k]$ two-point Padé form we have then according to (4.5).

$$g^- u_k + f^- v_k = \zeta^{-m}\hat{p}_n u_k + \zeta^{-m-1} p_n v_k = \zeta^{l-1} e_k^{(n)-} = O_-(\zeta^{l-1}).$$

Therefore,

$$p_{n+k} = \zeta \hat{p}_n u_k + p_n v_k = \zeta^{m+l} e_k^{(n)-} = O_-(\zeta^{m+l}),$$

i.e., $\partial p_{n+k} \le m+l$, and $e_k^{(n)-} = \zeta^{-m-l} p_{n+k}$. In view of $\partial \hat{p}_n \le m-1$, we have $\gamma_0^- = 0$ and from $\partial(\zeta \hat{p}_n u_k) \le m+k-1$ we obtain $\partial v_k \le k-1$, *i.e.*, $\beta_{k,k} = 0$. Moreover, from

$$g^+ u_k + f^+ v_k = \hat{e}_n u_k + e_n v_k = \zeta^{k+l} e_k^{(n)+} = O_+(\zeta^{k+l})$$

it follows that

$$e_{n+k} = \zeta^{-k-l}(\hat{e}_n u_k + e_n v_k) = e_k^{(n)+} = O_+(1).$$

Hence, $e_{n+k} = \hat{e}_k^{(n)+} \in \mathcal{L}_0$. From the definitions of p_n, q_n, e_n, $\hat{p}_n$, $\hat{q}_n$, and $\hat{e}_n$ one easily verifies that

$$hq_{n+k} - p_{n+k} = \zeta^{m+n+1}\zeta^{k+l}e_{n+k}.$$

This means that (p_{n+k}, q_{n+k}) is an $(m+l, n+k)$ Padé form of h, and that e_{n+k} is the corresponding residual.

(ii) The first part is proved by simply replacing l by $l-1$ and (u_k, v_k) by $(\hat{u}_k, \hat{v}_k)$ in (5.2). The final sentence follows by taking determinants in (5.3):

$$\det\begin{bmatrix} \hat{p}_{n+k} & p_{n+k} \\ \hat{q}_{n+k} & q_{n+k} \end{bmatrix} = \zeta \det\begin{bmatrix} \hat{p}_n & p_n \\ \hat{q}_n & q_n \end{bmatrix} \det\begin{bmatrix} \hat{u}_k & u_k \\ \hat{v}_k & v_k \end{bmatrix} \not\equiv 0.$$

□

The analogous recurrences for a two-point Padé table of data satisfying (4.3) are given in the following theorem.

THEOREM 5.2. *Let $(m,n) \in \mathbb{Z} \times \mathbb{N}^+$ satisfy $-n+1 \le m \le n$, and let (u_n, v_n) be a column-regular $[m;n]$ two-point Padé form with residual $(e_n^-; e_n^+)$ of a quadruple $(f^-, g^-; f^+, g^+)$ satisfying (4.3). Moreover, let $(\hat{u}_n, \hat{v}_n)$ be an $[m-1;n]$ two-point Padé form with residual $(\hat{e}_n^-; \hat{e}_n^+)$ of the same data.*

(i) If $(l,k) \in \mathbb{Z} \times \mathbb{N}^+$ satisfies $|l| < k$ or $|l| = k > 0$, and if $(u_k^{(n)}, v_k^{(n)})$ is an $[l;k]$ two-point Padé form with residual $(e_k^{(n)-}; e_k^{(n)+})$ of

$$(\zeta^{-1}e_n^-, \zeta^{-1}\hat{e}_n^-; e_n^+, \hat{e}_n^+), \tag{5.4}$$

then $\partial v_k^{(n)} \le k-1$ holds and the recurrence formula

$$\begin{bmatrix} u_{n+k} \\ v_{n+k} \\ \zeta^l e_{n+k}^- \\ \zeta^{k+l} e_{n+k}^+ \end{bmatrix} := \begin{bmatrix} \hat{u}_n & u_n \\ \hat{v}_n & v_n \\ \zeta^{-1}\hat{e}_n^- & e_n^- \\ \zeta^{-1}\hat{e}_n^+ & e_n^+ \end{bmatrix} \begin{bmatrix} \zeta u_k^{(n)} \\ v_k^{(n)} \end{bmatrix} \tag{5.5}$$

yields an $[m+l; n+k]$ two-point Padé form (u_{n+k}, v_{n+k}) of $(f^-, g^-; f^+, g^+)$ and its residual $(e_{n+k}^-; e_{n+k}^+)$, which is equal to $(e_k^{(n)-}, e_k^{(n)+})$.

(ii) If, moreover, $-k+1 \le l \le k$ and $(\hat{u}_k^{(n)}, \hat{v}_k^{(n)})$ is an $[l-1;k]$ two-point Padé form with residual $(\hat{e}_k^{(n)-}, \hat{e}_k^{(n)+})$ of (5.4), then $\partial \hat{v}_k^{(n)} \le k-1$ and we obtain from

$$\begin{bmatrix} \hat{u}_{n+k} & u_{n+k} \\ \hat{v}_{n+k} & v_{n+k} \\ \zeta^{l-1}\hat{e}_{n+k}^- & \zeta^l e_{n+k}^- \\ \zeta^{k+l-1}\hat{e}_{n+k}^+ & \zeta^{k+l} e_{n+k}^+ \end{bmatrix} := \begin{bmatrix} \hat{u}_n & u_n \\ \hat{v}_n & v_n \\ \zeta^{-1}\hat{e}_n^- & e_n^- \\ \zeta^{-1}\hat{e}_n^+ & e_n^+ \end{bmatrix} \begin{bmatrix} \zeta \hat{u}_k^{(n)} & \zeta u_k^{(n)} \\ \hat{v}_k^{(n)} & v_k^{(n)} \end{bmatrix} \tag{5.6}$$

additionally an $[m+l-1; n+k]$ two-point Padé form $(\hat{u}_{n+k}, \hat{v}_{n+k})$ and the corresponding residual $(\hat{e}_{n+k}^-; \hat{e}_{n+k}^+)$, which is equal to $(\hat{e}_k^{(n)-}, \hat{e}_k^{(n)+})$. The new two-point Padé form (u_{n+k}, v_{n+k}) is column-regular if and only if $(u_n^{(k)}, v_n^{(k)})$ is column-regular.

Proof. The proof is similar to the one of Theorem 5.1.

(i) From $\hat{u}_n, u_n \in \mathcal{P}_{n-1}$, and $\hat{v}_n, v_n \in \mathcal{P}_n$, it follows that $(u_{n+k}, v_{n+k}) \in \mathcal{P}_{n+k-1} \times \mathcal{P}_{n+k}$. By assumption, $(\hat{u}_n, \hat{v}_n)$ and (u_n, v_n) are $[m-1;n]$ and $[m;n]$ two-point Padé forms of the quadruple $(f^-, g^-; f^+, g^+)$, and $(u_k^{(n)}, v_k^{(n)})$ is an $[l;k]$ two-point Padé form of $(\zeta^{-1}e_n^-, \zeta^{-1}\hat{e}_n^-; e_n^+, \hat{e}_n^+)$. Note that the latter data satisfy (4.3) according to Lemma 4.2 (ii) and (iii). Therefore, we have

$$\begin{aligned} g^- u_{n+k} + f^- v_{n+k} &= \zeta(g^-\hat{u}_n + f^-\hat{v}_n)u_k^{(n)} + (g^- u_n + f^- v_n)v_k^{(n)} \\ &= \zeta^m(\zeta^{-1}\hat{e}_n^- u_k^{(n)} + \zeta^{-1}e_n^- v_k^{(n)}) \\ &= \zeta^{m+l-1}e_k^{(n)-} = O_-(\zeta^{m+l-1}) \end{aligned}$$

and

$$\begin{aligned} g^+ u_{n+k} + f^+ v_{n+k} &= \zeta(g^+\hat{u}_n + f^+\hat{v}_n)u_k^{(n)} + (g^+ u_n + f^+ v_n)v_k^{(n)} \\ &= \zeta^{m+n}(\hat{e}_n^+ u_k^{(n)} + e_n^+ v_k^{(n)}) \\ &= \zeta^{m+n+k+l}e_k^{(n)+} = O_+(\zeta^{m+n+k+l}). \end{aligned}$$

Hence, (u_{n+k}, v_{n+k}) is an $[m+k, n+l]$ two-point Padé form with residual $(e_{n+k}^-; e_{n+k}^+) = (e_k^{(n)-}; e_k^{(n)+})$. Note that as in Theorem 5.1 we always have $\partial v_k^{(n)} \leq k-1$, due to $\partial(\hat{e}_n^- u_k) \leq k-1$.

(ii) The first part follows from (i) by replacing l by $l-1$ and (u_n, v_n) by $(\hat{u}_n, \hat{v}_n)$. The second part is proved by taking determinants in (5.6):

$$\det \begin{bmatrix} \hat{u}_{n+k} & u_{n+k} \\ \hat{v}_{n+k} & v_{n+k} \end{bmatrix} = \zeta \det \begin{bmatrix} \hat{u}_n & u_n \\ \hat{v}_n & v_n \end{bmatrix} \det \begin{bmatrix} \hat{u}_k^{(n)} & u_k^{(n)} \\ \hat{v}_k^{(n)} & v_k^{(n)} \end{bmatrix} \not\equiv 0.$$

□

Recall that the data (5.1) always fulfills $\gamma_0^- = 0$ and $\phi_1^- \neq 0$. Therefore, Lemma 4.2 ensures that we can normalize $\hat{u}_k$ to be monic of degree $k-1$ (*i.e.*, $\hat{\alpha}_{k-1,k} = 1$) and v_k to be comonic (*i.e.*, $\beta_{0,k} = 1$). Then, if $\hat{q}_n$ is monic and q_n is comonic, the recursion (5.3) leads to a monic polynomial $\hat{q}_{n+k}$ and a comonic polynomial q_{n+k}. Hence, the recursion derived in Theorem 5.1 is compatible with the normalization. There is no need to renormalize the resulting Padé form. The same is true for the two-point Padé form recursion of Theorem 5.2.

6. Look-ahead strategies and numerical stability. For the development of stable algorithms for computing Padé approximants or solving Toeplitz systems it is not sufficient to work with column-regular Padé forms. In fact, column-regular Padé forms are useful only from a theoretical point of view. For finite precision arithmetic we need numerically stable algorithms and likewise for exact arithmetic we need versions that keep the memory requirement under control. Numerical stability should hold at least for well-conditioned problems, in which case forward and backward stability are equivalent. Hence, we set $m := 0$ and assume that our aim is to compute $(\hat{p}_N, \hat{q}_N)$ and/or (p_N, q_N) for some N for which, in view of the Yule-Walker equations (2.13), the matrix $\mathbf{T}_N := \mathbf{T}_{0;N}$ is well conditioned. Such generalizations of the Schur and Levinson algorithms can be based on well-column-regular Padé forms, which are defined as follows [22]. We denote the coefficient vectors of the normalized polynomials $\hat{q}_n$ and q_n by

$$\hat{\mathbf{q}}_n := [\begin{array}{cccc} \hat{\rho}_{0,n} & \cdots & \hat{\rho}_{n-1,n} & 1 \end{array}]^T, \quad \mathbf{q}_n := [\begin{array}{cccc} 1 & \hat{\rho}_{1,n} & \cdots & \hat{\rho}_{n,n} \end{array}]^T. \tag{6.1}$$

Definition. The normalized column-regular pair $(\hat{p}_n, \hat{q}_n)$, (p_n, q_n) of Padé forms is *well-column-regular* if $||\hat{\mathbf{q}}_n||$, $||\mathbf{q}_n|| <$ *Tol*(n) and $(|\hat{\varepsilon}_{n,n}| =)$ $|\pi_{0,n}| >$ *tol*(n). The index n is then also called well-column-regular. Here, $tol(n) > 0$ and $Tol(n) > 1$ denote given tolerances that are monotone increasing functions of n.

Column-regularity means that $||\mathbf{T}_n^{-1}||$ and $||\mathbf{T}_{n+1}^{-1}||$ are a priori bounded. In [22] we proved the following lemma.

LEMMA 6.1. *If n is well-column-regular, then*

$$\max\left\{||\mathbf{T}_n^{-1}||, ||\mathbf{T}_{n+1}^{-1}||\right\} < 2n\frac{[Tol(n)]^2}{tol(n)}.$$

Conversely, if $||\mathbf{T}_N|| < \tau$, $||\mathbf{T}_n^{-1}|| < \tau'$, and $||\mathbf{T}_{n+1}^{-1}|| < \tau'$, then

$$\max\{||\hat{\mathbf{q}}_n||, ||\mathbf{q}_n||\} < \sqrt{1 + (\tau\tau')^2}$$

and

$$|\hat{\varepsilon}_{n,n}| = |\varepsilon_{n,n}| > \frac{1}{\tau'} \max\{||\hat{\mathbf{q}}_n||, ||\mathbf{q}_n||\} \geq \frac{1}{\tau'}.$$

Since we want to assume that $||\mathbf{T}_N||$ is a priori bounded as well, which implies that the same bound holds for the norms of $\mathbf{T}_n$ and $\mathbf{T}_{n+1}$, it follows that the latter two matrices are well conditioned if n is well-column-regular. This yields an equivalent definition of a well-column-regular index, which was proposed in [20]. A fortiori, any well-column-regular Padé form is column-regular.

In each step of a Levinson or Schur algorithm based on Theorem 5.1 we need to check if $\hat{q}_{n+k}$ and q_{n+k} are part of a well-column-regular Padé form, and if the answer is negative, we have to repeat this check for the next k. If the above definition is applied, $||\hat{\mathbf{q}}_{n+k}||$, $||\mathbf{q}_{n+k}||$, and $|\pi_{0,n+k}|$ must be computed for all these values of k. In the Schur algorithm, these vectors are normally not available, however.

Following an approach first suggested in [20] and detailed in [22], we may instead use the results of the two-point Padé problems to control the process. The basic idea is that small coefficient vectors of the polynomials $\hat{u}_k^{(n)}$, $\hat{v}_k^{(n)}$, $u_k^{(n)}$, and $v_k^{(n)}$ in (5.3) guarantee that $||\hat{\mathbf{q}}_{n+k}||$ and $||\mathbf{q}_{n+k}||$ do not become very large. This gave rise to the following definition of well-column-regular index pairs of the two-point Padé problem used in the recursion [22].

DEFINITION. The column-regular index pair $(n;k)$ is *well-column-regular* if, for a suitable tolerance function $Tol(n;k) > 1$, the corresponding coefficient vectors $\hat{\mathbf{a}}^{(n)}$, $\hat{\mathbf{b}}^{(n)}$, $\mathbf{a}^{(n)}$, $\mathbf{b}^{(n)} \in \mathbb{C}^k$ of the two-point Padé forms $(\hat{u}_k^{(n)}, \hat{v}_k^{(n)})$, $(u_k^{(n)}, v_k^{(n)})$ normalized by $\hat{\alpha}_{k-1,k}^{(n)} = 1$ and $\hat{\beta}_{0,k}^{(n)}$, respectively, satisfy

$$\left\|\begin{bmatrix} \hat{\mathbf{a}}^{(n)} \\ \hat{\mathbf{b}}^{(n)} \end{bmatrix}\right\| < Tol(n;k), \quad \left\|\begin{bmatrix} \mathbf{a}^{(n)} \\ \mathbf{b}^{(n)} \end{bmatrix}\right\| < Tol(n;k), \tag{6.2}$$

and if

$$(\ |\hat{\varepsilon}_{n+k,n+k}| = \ )\ \ |\pi_{0,n+k}| > tol(n+k) \tag{6.3}$$

holds.

The new tolerance function $Tol(n;k)$ in (6.2) should be compatible with $Tol(n)$ in the sense that (6.2) implies that $n+k$ is a well-column-regular index if n is a well-column-regular index. Lemma 6.1 in [22] shows that such compatible tolerance

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functions exist. However, it seems difficult to prove the compatibility of practically useful such functions.

Finally, in view of (4.18) and (4.21), it is plausible that the condition (6.2) can be satisfied if the corresponding matrix $\mathbf{S}_{k-1}$ is sufficiently well conditioned and the right-hand sides of (4.18) and (4.21) are sufficiently small. Since, in our recurrences, these right-hand sides contain coefficients of the numerators and residuals, see (5.1), one can conclude from (2.10) that they are in fact small if the coefficient vectors $\hat{\mathbf{q}}_n$, $\mathbf{q}_n$ of $\hat{q}_n$ and q_n are sufficiently small, which we may assume since n is a well-column-regular index. (Note that p_n and e_n are both made up of sections of the Laurent series hq_n, and, likewise, $\hat{p}_n$ and $\hat{e}_n$ are extracted from $h\hat{q}_n$.)

In summary, a look-ahead strategy may be based on checking that $n+k$ is a well-column-regular index, or on checking that $(n;k)$ is a well-column-regular index pair, or on a direct estimate (or even the determination) of the condition number of $\mathbf{S}_{k-1}$. This leads to various versions of the algorithms, with different look-ahead overhead; see the discussion in §6 and §11 of [22].

7. Formally biorthogonal polynomials and matrix factorizations. It is well known that the classical Levinson and Schur algorithms yield an inverse LDU factorization and an ordinary LDU factorization, respectively, of the given Toeplitz matrix. The factors of the inverse factorization contain the coefficients of the Szegő polynomials. It is also known that the application of look-ahead leads to corresponding block factorizations [10, 17, 20, 22]. But so far, our algorithms only produce the first column of each block of the block triangular factors. Here, we want to show how to compute the other columns efficiently. We restrict ourselves to the Levinson case, *i.e.*, the inverse block LDU factorization. Analogous recursions hold in the Schur case. They are given in [22], where the efficient construction of the block diagonal is also discussed.

Given $h \in \mathcal{L}$, or, equivalently, the doubly infinite sequence $\{\mu_k\}_{k=-\infty}^{\infty}$ of coefficients, we define a sesquilinear functional $\langle\cdot,\cdot\rangle$ on $\mathcal{P}\times\mathcal{P}$ by its values

$$\langle\zeta^i,\zeta^j\rangle := \mu_{i-j}, \quad (i,j)\in\mathbb{N}\times\mathbb{N}. \tag{7.1}$$

For arbitrary polynomials s and t of degree less than n represented by

$$s(\zeta) =: \sum_{j=0}^{n}\sigma_j\zeta^j, \quad t(\zeta) =: \sum_{j=0}^{n}\tau_j\zeta^j, \tag{7.2}$$

we set $\sigma_j = \tau_j = 0$ for $j > n$ and introduce the infinite coefficient vectors

$$\mathbf{s} := [\ \sigma_0 \quad \cdots \quad \sigma_n \quad 0 \quad \cdots\ ]^T, \quad \mathbf{t} := [\ \tau_0 \quad \cdots \quad \tau_n \quad 0 \quad \cdots\ ]^T. \tag{7.3}$$

Then, it is well known and easily verified that

$$\langle s,t\rangle = \sum_{i,j=0}^{\infty}\overline{\sigma_i}\mu_{i-j}\tau_j. = \mathbf{s}^H\mathbf{T}\,\mathbf{t}, \tag{7.4}$$

where $\mathbf{T} := [\mu_{i-j}]_{i,j=0}^{\infty}$ is the Toeplitz operator with the symbol $h(\zeta) = \sum\mu_k\zeta^k$.

Definition. $s\in\mathcal{P}_n\backslash\mathcal{P}_{n-1}$ is called an nth *left formally biorthogonal polynomial* (LOP), and $t\in\mathcal{P}_n\backslash\mathcal{P}_{n-1}$ is called an nth *right formally biorthogonal polynomial* (ROP) if

$$\langle s,\zeta^j\rangle = 0, \qquad j=0,\ldots,n-1, \tag{7.5}$$

$$\langle\zeta^i,t\rangle = 0, \qquad i=0,\ldots,n-1, \tag{7.6}$$

respectively. An nth LOP or ROP is said to be *regular* if it is uniquely determined up to scaling; otherwise, it is *singular*.

If we further define the conjugate reflected polynomial $s^\star$ of an nth LOP s by

$$s^\star(\zeta) := \zeta^n \overline{s}(\zeta^{-1}) = \sum_{i=0}^{n} \overline{\sigma}_{n-i}\zeta^i, \tag{7.7}$$

then (7.5) and (7.6) can be written as

$$\Pi_{1:n}(hs^\star) = 0 \quad \text{and} \quad \Pi_{0:n-1}(ht) = 0, \tag{7.8}$$

respectively. Thus, the conjugate reflected polynomial $s^\star$ of an nth LOP s is equal to the second member q_n of a $(0, n)$ Padé form (p_n, q_n) of h, while an nth ROP t is equal to a second member $\hat{q}_n$ of a $(-1, n)$ Padé form $(\hat{p}_n, \hat{q}_n)$ [8, 7]. From now on we therefore denote an nth LOP by $q_n^\star$ and an nth ROP by $\hat{q}_n$. Since both the LOP and the ROP need to have exact degree n, they can be normalized to be monic. Then the conditions (7.5) and (7.6), when expressed in terms of the polynomial coefficients, become exactly the Yule-Walker equations (2.13) with $m = 0$. The required uniqueness of a regular normalized LOP and ROP is thus seen to be equivalent to the nonsingularity of $\mathbf{T}_n := \mathbf{T}_{0;n}$. In particular, it follows that the nth LOP is regular if and only if the nth ROP is. Moreover, from the block structure of the Padé table it follows that they are regular if and only if the $(0, n)$ Padé approximant p_n/q_n lies in the first column or the first row of its block. Such a Padé approximant is also characterized by being different from its upper-left neighbor. In this case, the Padé form (p_n, q_n) is called *regular* also [9, 20].

In the generic case where $q_n^\star$ and $\hat{q}_n$ are regular for every n, these polynomials are called *Szegő polynomials*. When $\mathbf{T}$ is Hermitian, $q_n^\star = \hat{q}_n$. Szegő only considered the special case where $\mathbf{T}$ is additionally positive definite and the polynomials are classical orthogonal polynomials.

In the context of this paper we have been dealing only with a subset of the regular LOPs and ROPs. First, our algorithms (if applied with $m = 0$), only generate *column-regular* Padé forms (p_n, q_n) and their upper neighbors $(\hat{p}_n, \hat{q}_n)$. According to Lemma 3.1 this means that in addition to $\mathbf{T}_n$ also $\mathbf{T}_{n+1}$ must be nonsingular. Moreover, for stability reasons, these matrices should not be close to singular, but well conditioned, in which case we called the two Padé forms a *well-column-regular* pair. The index n was also said to be well-column-regular.

In the following we let $\{n_j\}_{j=0}^{J}$ (with $J \le \infty$) be such a subsequence of well-column-regular indices. For the other indices we introduce *inner* LOPs and ROPs as follows.

Definition. For $n_j = n < n + k < n_{j+1}$, an $(n + k)$th *inner* LOP $q_{n+k}^\star$ and an $(n + k)$th *inner* ROP $\hat{q}_{n+k}$ are any polynomials of exact degree $n + k$ satisfying

$$\langle q_{n+k}^\star, \zeta^i\rangle = 0, \qquad i = 0, \ldots, n, \tag{7.9}$$

$$\langle \zeta^i, \hat{q}_{n+k}\rangle = 0, \qquad i = 0, \ldots, n, \tag{7.10}$$

respectively.

Note that the column-regular LOP and ROP with index $n = n_j$ satisfy the biorthogonality conditions in (7.9) and (7.10), respectively, except for $i = n_j$. Moreover, if an inner LOP and an inner ROP with exact degree $n_j + 1$ exist (and we will see soon that they do), then they are still regular, but, in general, not column-regular.

In fact, in Fig. 1, where the exactly singular blocks are shown, it is evident that each first inner pair lies in the first column of a singular block; hence, this inner pair is not column-regular, but both (p_n, q_n) and $(\hat{p}_n, \hat{q}_n)$ are regular Padé forms.

Our next aim is to derive formulas for computing inner formally biorthogonal polynomials from the last pair of well-column-regular ones. First, we present two technical lemmas:

LEMMA 7.1. *Let $h \in \mathcal{L}$ and the associated sesquilinear functional $\langle .,. \rangle$ specified by (7.1) be given, and let $k, n \geq 0$. For $q_{n+k} \in \mathcal{P}_{n+k}$ and $q^{\star}_{n+k}(\zeta^{-1}) := \zeta^{n+k} q_{n+k}(\zeta)$, the following statements are equivalent:*

(i) $\langle q^{\star}_{n+k}, \zeta^i \rangle = 0$ *for* $i = 0, \ldots, n$;

(ii) $\Pi_{k:n+k}(hq_{n+k}) = 0$;

(iii) *there exists* $p_{n+k} \in \mathcal{L}^*_{k-1}$ *such that*

$$hq_{n+k} - p_{n+k} = O_+(\zeta^{n+k+1}). \tag{7.11}$$

Proof. All three statements translate into $\sum_{\ell=0}^{n+k} \rho_{\ell,n+k} \mu_{n+k-i-\ell} = 0$, $i = 0, \ldots, n$. □

LEMMA 7.2. *Let $h \in \mathcal{L}$ and the associated sesquilinear functional $\langle .,. \rangle$ specified by (7.1) be given, and let $k, n \geq 0$. For $\hat{q}_{n+k} \in \mathcal{P}_{n+k}$ the following statements are equivalent:*

(i) $\langle \zeta^i, \hat{q}_{n+k} \rangle = 0$ *for* $i = 0, \ldots, n$;

(ii) $\Pi_{0:n}(h\hat{q}_{n+k}) = 0$;

(iii) *there exists* $\hat{p}_{n+k} \in \mathcal{L}^*_{-1}$ *such that*

$$h\hat{q}_{n+k} - \hat{p}_{n+k} = O_+(\zeta^{n+1}). \tag{7.12}$$

Proof. Here, the three statements are equivalent to $\sum_{\ell=0}^{n+k} \mu_{i-\ell} \hat{\rho}_\ell = 0$, $i = 0, \ldots, n$. □

From (7.12) we see that $(\hat{p}_{n+k}, \hat{q}_{n+k})$ can be thought of as a *underdetermined* $(-1, n)$ Padé form when $k > 1$: instead of $O_+(\zeta^{n+k})$ we only require $O_+(\zeta^{n+1})$. Likewise, (7.11) specifies another type of underdetermined $(0, n)$ Padé form when $k > 1$: here, the condition $p_{n+k} \in \mathcal{L}^*_{k-1}$ relaxes the usual requirement $p_{n+k} \in \mathcal{L}^*_0$ of a $(0, n)$ Padé form.

Next we give the desired update formulas for the inner polynomials.

THEOREM 7.3. *Let (p_n, q_n) be a column-regular $(0, n)$ Padé form of h, and let e_n be its residual. Moreover, let $(\hat{p}_n, \hat{q}_n)$ be a $(-1, n)$ Padé form of h with residual $\hat{e}_n$.*

(*i*) *If, for $k > 0$, $u^{(n)}_k \in \mathcal{P}_{k-1}$ is a solution of*

$$\hat{e}_n u^{(n)}_k + e_n = O_+(\zeta^k), \tag{7.13}$$

and if we define

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \end{bmatrix} := \begin{bmatrix} \zeta\hat{p}_n & p_n \\ \zeta\hat{q}_n & q_n \end{bmatrix} \begin{bmatrix} u^{(n)}_k \\ 1 \end{bmatrix}, \tag{7.14}$$

then $p_{n+k} \in \mathcal{L}^{\star}_{k-1}$, $q_{n+k} \in \mathcal{P}_{n+k}$, $q_{n+k}(0) \neq 0$, and the condition (7.11) *is satisfied.*

(*ii*) *If, for $k > 0$, $\hat{v}^{(n)}_k \in \mathcal{P}_{k-1}$ is a solution of*

$$\zeta^k \hat{p}_n + p_n \hat{v}^{(n)}_k = O_-(\zeta^{-1}), \tag{7.15}$$

and if we define

$$\begin{bmatrix} \hat{p}_{n+k} \\ \hat{q}_{n+k} \end{bmatrix} := \begin{bmatrix} \zeta\hat{p}_n & p_n \\ \zeta\hat{q}_n & q_n \end{bmatrix} \begin{bmatrix} \zeta^{k-1} \\ \hat{v}_k^{(n)} \end{bmatrix}, \tag{7.16}$$

then $\hat{p}_{n+k} \in \mathcal{L}^\star_{-1}$, $\hat{q}_{n+k} \in \mathcal{P}_{n+k}$, $\partial\hat{q}_{n+k} = n+k$, *and the condition* (7.12) *is satisfied.*

Proof. (i) By (7.14), clearly $q_{n+k} \in \mathcal{P}_{n+k}$. We have $q_n(0) \neq 0$, since (p_n, q_n) is a column-regular $(0, n)$ Padé form of h. Thus, from (7.14) we also conclude that $q_{n+k}(0) = q_n(0) \neq 0$. Due to the column-regularity of (p_n, q_n), we have $\partial p_n = 0$ and $\partial\hat{p}_n \leq -1$, which leads to $p_{n+k} \in \mathcal{L}^*_{k-1}$. Moreover,

$$\begin{aligned} hq_{n+k} - p_{n+k} &= h(\zeta\hat{q}_n u_k^{(n)} + q_n) - (\zeta\hat{p}_n u_k^{(n)} + p_n) \\ &= \zeta^{n+1}(\hat{e}_n u_k^{(n)} + e_n). \end{aligned}$$

This shows that (7.11) follows from (7.13).

(ii) From (7.16) it follows immediately that $\partial\hat{q}_{n+k} = n+k$, since $\partial\hat{q}_n = n$ and $\partial q_n \leq n$. Additionally, we see from (7.15) and (7.16) that $\hat{p}_{n+k} \in \mathcal{L}^*_{-1}$. Finally, by the column-regularity of (p_n, q_n), we obtain

$$\begin{aligned} h\hat{q}_{n+k} - \hat{p}_{n+k} &= h(\zeta^k\hat{q}_n + q_n\hat{v}_k^{(n)}) - (\zeta^k\hat{p}_n + p_n\hat{v}_k^{(n)}) \\ &= \zeta^{n+1}(\zeta^{k-1}\hat{e}_n + e_n\hat{v}_k^{(n)}), \end{aligned}$$

which implies (7.12). ◻

From the Lemmas 7.1 and 7.2 it follows that Theorem 7.3 yields in fact inner LOPs and ROPs. As mentioned before, the first inner pair consists here of regular Padé forms; see Fig. 1.

COROLLARY 7.4. *Let the assumptions of Theorem* 7.3 *be satisfied, let* q_{n+k} *and* $\hat{q}_{n+k}$ *be given by the update formulas* (7.14) *and* (7.16), *respectively, and let* $q^\star_{n+k}(\zeta) := \zeta^{n+k}q_{n+k}(\zeta)$ *as in Lemmas 7.1. Then, for* $k > 0$, *the biorthogonality properties* (7.9)-(7.10) *hold. Hence, for* $0 < k < n_{j+1} - n_j$, *the polynomials* $q^\star_{n+k}$ *and* $\hat{q}_{n+k}$ *are inner LOPs and ROPs, respectively. Moreover, the first such pair,* $q^\star_{n+1}$ *and* $\hat{q}_{n+1}$ *even consists of a regular* $(n+1)$*st LOP and a regular* $(n+1)$*st ROP.*

Proof. (7.9) is a consequence of $p_{n+k} \in \mathcal{L}^*_{k-1}$, (7.11), and Lemma 7.1. Similarly, (7.10) follows from $\hat{p}_{n+k} \in \mathcal{L}^*_{-1}$, (7.12), and Lemma 7.2. ◻

We would like to stress that the column-regularity of (p_n, q_n) implies that solutions $u_k^{(n)}$, $\hat{v}_k^{(n)} \in \mathcal{P}_{k-1}$ of (7.13) and (7.15) exist. To be precise, if

$$u_k^{(n)} =: \sum_{j=0}^{k-1} \gamma_j^{(n)}\zeta^j, \qquad \hat{v}_k^{(n)} =: \sum_{j=0}^{k-1} \hat{\gamma}_{k-j-1}^{(n)}\zeta^j, \tag{7.17}$$

then the coefficients $\gamma_0^{(n)}, \ldots, \gamma_{k-1}^{(n)}$ solve the first k equations of the infinite lower triangular Toeplitz system

$$\begin{bmatrix} \hat{\varepsilon}_{n,n} & & & \\ \vdots & \ddots & & \\ \hat{\varepsilon}_{n+k-1,n} & \cdots & \hat{\varepsilon}_{n,n} & \\ \vdots & & & \ddots \end{bmatrix} \begin{bmatrix} \gamma_0^{(n)} \\ \vdots \\ \gamma_{k-1}^{(n)} \\ \vdots \end{bmatrix} = - \begin{bmatrix} \varepsilon_{n,n} \\ \vdots \\ \varepsilon_{n+k-1,n} \\ \vdots \end{bmatrix}, \tag{7.18}$$

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and the coefficients $\hat{\gamma}_0^{(n)}, \ldots, \hat{\gamma}_{k-1}^{(n)}$, which are indexed in reverse order, solve the first k equations of

$$\begin{bmatrix} \pi_{0,n} & & & \\ \vdots & \ddots & & \\ \pi_{k-1,n} & \cdots & \pi_{0,n} & \\ \vdots & & & \ddots \end{bmatrix} \begin{bmatrix} \hat{\gamma}_0^{(n)} \\ \vdots \\ \hat{\gamma}_{k-1}^{(n)} \\ \vdots \end{bmatrix} = - \begin{bmatrix} \hat{\pi}_{1,n} \\ \vdots \\ \hat{\pi}_{k,n} \\ \vdots \end{bmatrix}. \tag{7.19}$$

These linear systems are nonsingular, since for a column-regular $(0, n)$ Padé form, $\hat{e}_n(0) = \hat{\varepsilon}_{n,n} \neq 0$ and $\partial p_n = 0$, *i.e.*, $\pi_{0,n} \neq 0$. Note that the coefficients in (7.17) and (7.19) do not depend on k. It is just the number of coefficients $\gamma_i^{(n)}$ and $\hat{\gamma}_i^{(n)}$ that accounts for the dependence on k. This is due to the triangular Toeplitz structure of the two linear systems, which is also responsible for the particularly simple recurrences for the polynomials $u_k^{(n)}$ and $\hat{v}_k^{(n)}$: for the coefficients we have

$$\begin{aligned} \gamma_0^{(n)} &= -\varepsilon_{n,n}/\hat{\varepsilon}_{n,n}, \\ \gamma_j^{(n)} &= -\left(\varepsilon_{n+j,n} + \textstyle\sum_{i=0}^{j-1} \hat{\varepsilon}_{n+j-i,n}\gamma_i^{(n)}\right)/\hat{\varepsilon}_{n,n} \qquad \text{for } j = 1, \ldots, k-1, \end{aligned} \tag{7.20}$$

$$\begin{aligned} \hat{\gamma}_0^{(n)} &= -\hat{\pi}_{1,n}/\hat{\pi}_{0,n}, \\ \hat{\gamma}_j^{(n)} &= -\left(\hat{\pi}_{j+1,n} + \textstyle\sum_{i=0}^{j-1} \pi_{j-i,n}\hat{\gamma}_i^{(n)}\right)/\pi_{0,n} \qquad \text{for } j = 1, \ldots, k-1. \end{aligned} \tag{7.21}$$

Hence, for the polynomials $u_k^{(n)}$ and $\hat{v}_k^{(n)}$, the following recurrences hold:

$$\begin{aligned} u_1^{(n)} &= \gamma_0^{(n)}, \qquad & u_k^{(n)} &= u_{k-1}^{(n)} + \gamma_{k-1}^{(n)}\zeta^{k-1} \qquad && \text{for } k = 2, 3, \ldots, \\ \hat{v}_1^{(n)} &= \hat{\gamma}_0^{(n)}, \qquad & \hat{v}_k^{(n)} &= \hat{\gamma}_{k-1}^{(n)} + \zeta\hat{v}_{k-1}^{(n)} \qquad && \text{for } k = 2, 3, \ldots. \end{aligned} \tag{7.22}$$

Inserting this into the update formulas of Theorem 7.3 yields simple recurrences for the inner polynomials also:

THEOREM 7.5. *Let the assumptions of Theorem 7.3 be satisfied and let, with* $n = n_j$,

$$q_{n+1} = \zeta\hat{q}_n\gamma_0^{(n)} + q_n \quad \text{and} \quad \hat{q}_{n+1} = \zeta\hat{q}_n + q_n\hat{\gamma}_0^{(n)}. \tag{7.23}$$

Then, $q_{n+1}^{\star}$ *is a regular* $(n+1)$*st LOP and* $\hat{q}_{n+1}$ *is a regular* $(n+1)$*st ROP. Moreover, for the inner LOPs and ROPs of Theorem 7.3 and Corollary 7.4, the following recurrences hold:*

$$\begin{aligned} q_{n+k} &= \zeta^{k-1}\hat{q}_n\gamma_{k-1}^{(n)} + q_{n+k-1} \qquad && \text{for } k = 2, \ldots, n_{j+1} - n_j - 1, \\ \hat{q}_{n+k} &= \zeta\hat{q}_{n+k-1} + q_n\hat{\gamma}_{k-1}^{(n)} \qquad && \text{for } k = 2, \ldots, , n_{j+1} - n_j - 1. \end{aligned} \tag{7.24}$$

8. A superfast algorithm. As mentioned before, depending on what exactly is computed, the recurrences (5.3) of Theorem 5.1 give rise to both a look-ahead Schur and a look-ahead Levinson algorithm for computing an (m, N) Padé form of h. For the generalization of Levinson's algorithm only the denominators of the Padé forms are used, while the generalization of Schur's algorithm requires computing residuals and numerators of the Padé forms. We do not discuss the details of the $O(N^2)$ algorithms

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here, since they can be found in [22]. But additionally, the recurrences derived in §5 also lead to superfast $O(N \log^2 N)$ algorithms, and such an algorithm is what we want to discuss here. It differs from the one that has been outlined in [22] in that it is implemented in just one procedure that calls itself recursively.

A superfast algorithm is a variant of the Schur algorithm; it mainly works with residuals and numerators of Padé forms. The basic idea is the following. Let us assume that $\{n_j\}_{j=0}^J$ (with $J \leq \infty$ and $n_J = N$) is a subsequence of well-column-regular indices, and, as before, let $h_j := n_{j+1} - n_j$. We only compute Padé forms for such indices. From (5.3) we have

$$\begin{bmatrix} \hat{p}_{n_J} & p_{n_J} \\ \hat{q}_{n_J} & q_{n_J} \\ \zeta^{n_J-1}\hat{e}_{n_J} & \zeta^{n_J} e_{n_J} \end{bmatrix} \tag{8.1a}$$

$$= \begin{bmatrix} \hat{p}_{n_{J-1}} & p_{n_{J-1}} \\ \hat{q}_{n_{J-1}} & q_{n_{J-1}} \\ \zeta^{n_{J-1}-1}\hat{e}_{n_{J-1}} & \zeta^{n_{J-1}} e_{n_{J-1}} \end{bmatrix} \begin{bmatrix} \zeta\hat{u}_{h_{J-1}}^{(n_{J-1})} & \zeta u_{h_{J-1}}^{(n_{J-1})} \\ \hat{v}_{h_{J-1}}^{(n_{J-1})} & v_{h_{J-1}}^{(n_{J-1})} \end{bmatrix}$$

$$= \begin{bmatrix} \hat{p}_{n_0} & p_{n_0} \\ \hat{q}_{n_0} & q_{n_0} \\ \zeta^{n_0-1}\hat{e}_{n_0} & \zeta^{n_0} e_{n_0} \end{bmatrix} \prod_{j=0}^{J-1} \begin{bmatrix} \zeta\hat{u}_{h_j}^{(n_j)} & \zeta u_{h_j}^{(n_j)} \\ \hat{v}_{h_j}^{(n_j)} & v_{h_j}^{(n_j)} \end{bmatrix}. \tag{8.1b}$$

Hence, we can compute the numerators, denominators, and residuals of a well-column-regular Padé form by evaluating the product of 2×2 matrices whose entries are polynomials of degrees $h_j - 1$. Of course, using the Padé conditions (2.10), we could instead compute the numerators and residuals from the denominators, but this involves convolutions that we want to avoid here. Note that when $n_0 = 0$ (which is normally the case), and when we replace μ_k by 0 if $k < m - N$ or $k > m + N$ (because these coefficients are irrelevant for the denominators of the $(m-1, N)$ and (m, N) Padé forms), then the left matrix in (8.1b) is just

$$\begin{bmatrix} \hat{p}_0 & p_0 \\ \hat{q}_0 & q_0 \\ \zeta^{-1}\hat{e}_0 & e_0 \end{bmatrix} = \begin{bmatrix} \Pi_{m-N:m-1}\, h & \Pi_{m-N:m}\, h \\ 1 & 1 \\ \zeta^{-1}\Pi_{m:m+N}\, h & \Pi_{m+1:m+N}\, h \end{bmatrix}. \tag{8.2}$$

Note that all the coefficients of the Laurent polynomials in this matrix are given coefficients of h.

To achieve a superfast algorithm, we build up the product in (8.1b) according to a binary tree, starting on one side, at $j = 0$. Since the factors of this product, which contain the low-degree two-point Padé forms, are not known in advance, they need to be determined during the process. To compute these two-point Padé forms, the numerators and residuals of the already determined Padé forms are required; see Theorem 5.1. These numerators and residuals could also be updated from step to step, namely by making use of the first and third row of (8.1b); see (5.3). However, to do this for each j would be too costly and would conflict with the evaluation of the product via the binary tree. However, we can think of these numerators and residuals as residuals of two-point Padé forms, and then refer to Theorem 5.2 instead. Then we actually have to solve a binary tree of two-point Padé problems; on those levels of the tree where there are many of these problems, they are small and depend only on few data. Here is a summary of this algorithm:

SUPERFAST LOOK-AHEAD SCHUR ALGORITHM:
Computes the denominators of an $(m;N)$ and an $(m-1;N)$ Padé form of h.

A1) Set $n := 0$; increase n until it is a well-column-regular index;
set $n_0 := n$;
A2) solve (2.13) to obtain $\hat{q}_{n_0}$ and q_{n_0};
A3) evaluate

$$\hat{p}_{n_0} := \Pi_{m-N+n_0:m-1}\, h\hat{q}_{n_0}, \quad p_{n_0} := \Pi_{m-N+n_0:m}\, hq_{n_0},$$

and

$$\hat{e}_{n_0} := \Pi_{0:N-n_0}\, \zeta^{-m-n_0} h\hat{q}_{n_0}, \quad e_{n_0} := \Pi_{0:N-n_0-1}\, \zeta^{-m-n_0-1} hq_{n_0}.$$

A4) $[n, \hat{u}_n, \hat{v}_n, u_n, v_n, n_{\text{tot}}, \mathit{flag}]$
$:= \text{COLDAC2}(\mathit{true}, n_0, N, \zeta^{-m-1}p_{n_0}, \zeta^{-m}\hat{p}_{n_0}, e_{n_0}, \hat{e}_{n_0}, n_0);$
A5) if $n_{\text{tot}} = N$

$$\begin{bmatrix} \hat{q}_N & q_N \end{bmatrix} := \begin{bmatrix} \hat{q}_{n_0} & q_{n_0} \end{bmatrix} \begin{bmatrix} \zeta\hat{u}_n & \zeta u_n \\ \hat{v}_n & v_n \end{bmatrix},$$

else
stop, the problem is ill-conditioned
end

PROCEDURE COLDAC2:
For minimal $N \in [\overline{N}, \underline{N}]$, and f^-, g^-, f^+, g^+ satisfying (4.3) or (4.4), a well-column-regular pair of two-point Padé forms is computed. If *dac* is true, than a divide and conquer strategy is applied; otherwise a linear system is solved.

$[N, \hat{u}_N, \hat{v}_N, u_N, v_N, n_{\text{tot}}, \mathit{flag}] := \text{COLDAC2}(\mathit{dac}, \underline{N}, \overline{N}, f^-, g^-, f^+, g^+, n_{\text{tot}});$
if *dac* and $\underline{N} \geq 2$
B1)
$[n, \hat{u}_n, \hat{v}_n, u_n, v_n, n_{\text{tot}}, \mathit{flag}]$
$:= \text{COLDAC2}(\mathit{true}, \lfloor \underline{N}/2 \rfloor, \overline{N}-1, f^-, g^-, f^+, g^+, n_{\text{tot}});$
B2) if *flag* and $n = 0$
$[N, \hat{u}_N, \hat{v}_N, u_N, v_N, n_{\text{tot}}, \mathit{flag}] := \text{COLDAC2}(\mathit{false}, \underline{N}, \overline{N}, f^+, g^+, f^-, g^-, n_{\text{tot}});$
return
end if;
B3) evaluate

$$\begin{aligned} \hat{e}_n^- &:= \Pi_{-\overline{N}+n:0}\, \zeta^2(g^-\hat{u}_n + f^-\hat{v}_n), \\ \hat{e}_n^+ &:= \Pi_{0:\overline{N}-n}\, \zeta^{-n+1}(g^+\hat{u}_n + f^+\hat{v}_n), \\ e_n^- &:= \Pi_{-\overline{N}+n:0}\, \zeta(g^-u_n + f^-v_n), \\ e_n^+ &:= \Pi_{0:\overline{N}-n}\, \zeta^{-n}(g^+u_n + f^+v_n); \end{aligned}$$

B4) $[k, \hat{u}_k^{(n)}, \hat{v}_k^{(n)}, u_k^{(n)}, v_k^{(n)}, n_{\text{tot}}, \mathit{flag}] :=$
$\text{COLDAC2}(\mathit{true}, \underline{N}-n, \overline{N}-n, \zeta^{-1}\hat{e}_n^-, \zeta^{-1}e_n^-, \hat{e}_n^+, e_n^+, n_{\text{tot}});$
if *flag* and $k = 0$

$N := n_{\rm tot}$;
return
end if;
B5) $N := n + k$, *flag* := *false*;

$$\begin{bmatrix} \hat{u}_{n+k} & u_{n+k} \\ \hat{v}_{n+k} & v_{n+k} \end{bmatrix} := \begin{bmatrix} \hat{u}_n & u_n \\ \hat{v}_n & v_n \end{bmatrix} \begin{bmatrix} \zeta \hat{u}_k^{(n)} & \zeta u_k^{(n)} \\ \hat{v}_k^{(n)} & v_k^{(n)} \end{bmatrix},$$

return
else
C1) $k := \underline{N}$;
while $(n_{\rm tot}; k)$ is not a well-column-regular index pair and $k < \overline{N}$
set $k := k + 1$
end while;
if $(n_{\rm tot}; k)$ is a well-column-regular index pair
flag := *false*, $N := k$, $n_{\rm tot} := n_{\rm tot} + k$;
solve (4.18) and (4.21) to obtain $\hat{u}_N, \hat{v}_N, u_N, v_N$
else
$N := 0$, *flag* := *true*
end if;
return
end if

To discuss the computational work, let us first assume that $n_j = j$, $j = 0, \ldots, J$, *i.e.*, every index is well-column-regular, and that $N = n_J$ is a power of 2. Then a call to COLDAC2 splits the problem into two problems of half the size. There are $\log_2 N$ steps of reduction before we finally end up with N system of size one. On level ℓ, where ℓ problems of size N/ℓ are solved, the work inside the procedure COLDAC2 is of order $O((N/\ell)\log(N/\ell))$ if all polynomial multiplications are done by FFT techniques. Hence, the total on level ℓ is $O(N \log(N/\ell)) = O(N \log N)$. Summing over ℓ from 1 to $log_2 N$ yields a total complexity of $O(N \log^2 N)$.

If look-ahead steps occur, then a call to COLDAC2 may not split the problem into two tasks of equal size. Instead it will find a splitting into two well-conditioned problems of approximately half the size. As long as the look-ahead step size remains bounded independent of N, the order of complexity of the algorithm is not affected by look-ahead.

It is worth mentioning that in the generic case, *i.e.*, without look-ahead, the algorithm reduces to de Hoog's algorithm [14]. Since the look-ahead overhead is small, not only the order of complexity but the actual number of operations and the memory requirement of our generalization should be roughly the same as for de Hoog's algorithm.

Note also that the superfast algorithm presented in [22] differs in one point. There, we compute $\approx \log_2 N$ column-regular pairs $\hat{q}_n, q_n$ (namely, in the absence of look-ahead steps for every $n = 2^\ell$, $\ell = 1, \ldots, \log_2 N$), while the algorithm proposed here yields only $\hat{q}_N, q_N$. For the algorithm in [22], we therefore had to cope with two types of recursive procedures, one for computing the Padé forms, the other for computing the two-point Padé forms. Thus, the algorithm proposed here reduces the programming effort. The two versions are mathematically equivalent; numerically, they are not identical, but the difference in numerical results will normally be very small.

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