Further optimized look-ahead recurrences for adjacent rows in the Padé table and Toeplitz matrix factorizations

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Dedicated to Prof. William B. Gragg on the occasion of his 60th birthday

Abstract

In a recent paper, we introduced a new look-ahead algorithm for recursively computing Padé approximants. This algorithm generates a subsequence of the Padé approximants on two adjacent rows (defined by fixed numerator degree) of the Padé table. Its two basic versions reduce to the classical Levinson and Schur algorithms if no look-ahead is required. In this paper, we show that the computational overhead of the look-ahead steps in the $O(N^2)$ versions of the look-ahead Levinson and the look-ahead Schur type algorithm can be further reduced.

If the algorithms are used to solve Toeplitz systems of equations $\mathbf{Tx} = \mathbf{b}$, then the corresponding block LDU decompositions of $\mathbf{T}^{-1}$ or $\mathbf{T}$, respectively, can be found with less computational effort than with any other look-ahead algorithm available today.

Key words: Padé approximation, row recurrence, fast algorithm, sawtooth recurrence, look-ahead, Toeplitz matrix, Levinson algorithm, Schur algorithm, biorthogonal polynomials.

1 Introduction

In this paper, we improve the algorithm we proposed recently for computing a $(0, N)$ Padé form of a formal Laurent series h with complex coefficients [15]. This variant and others described previously in [12–14] construct regular or column-regular Padé forms from regular or column-regular Padé forms of lower denominator degree. The basic ingredient to proceed along adjacent rows in the Padé table is to multiply both members of a regular pair by polynomials

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of low degree. To be more precise, these polynomials are two-point Padé forms of residuals and numerators of the regular pair.

Here we describe a different approach. We have shown that the gaps between two regular pairs of Padé forms can be filled by so-called left and right underdetermined Padé forms, which correspond to inner formally biorthogonal polynomials. However, in our algorithms [12–15], these underdetermined Padé forms were constructed solely to complete the block LDU or the inverse block LDU decomposition of a Toeplitz matrix, but were not used for anything else. This is exactly, what we want to change here. We build the next regular pair with the help of underdetermined Padé forms. Since we then no longer have recurrences based on multiplication of polynomials, we lose the option to extend the fast $O(N^2)$ algorithms to superfast $O(N \log^2 N)$ algorithms. This disadvantage is compensated by the fact that the new algorithm has less overhead than any other known look-ahead algorithm that computes the complete factorization of a Toeplitz matrix. Moreover, superfast algorithms are faster only for sufficiently large dimensions N, and hence, stable fast algorithms are still of interest. Instead of products of polynomials, the new recurrences only involve linear combinations of previous (underdetermined) Padé forms or shifted copies of those.

The idea of using inner formally orthogonal or biorthogonal polynomials in different kinds of look-ahead algorithms is by far not new. It was used in the look-ahead Lanczos process [5], the look-ahead Hankel solver [8] and its block version [23], and the look-ahead Toeplitz solvers [4,7]. However, to the best of our knowledge it seems to be new to use underdetermined Padé forms to construct recurrences in non-normal Padé tables. We will show that the Padé approach can help to find more efficient recurrences. To convince the reader of this statement, we reinterpret the algorithms proposed by Freund and Zha [7] and by Freund [4] in terms of Padé approximation. We will see that these algorithms can be improved by exploiting classical recurrences known in the Padé literature. A nice overview of relations between formally biorthogonal polynomials, Padé approximation, Hankel, and Toeplitz matrices in *exact arithmetic* was recently written by Bultheel and van Barel [1].

A benefit of looking into algorithms for Toeplitz matrix factorization or for constructing formally biorthogonal polynomials from the Padé point of view is that the same arguments can be used to derive recurrences for Levinson and Schur type algorithms. We would like to stress that in order to establish the recurrences no deep understanding of Padé approximation is necessary, except for the fact that (m, n) Padé forms exist for any pair of integers (m, n) with nonnegative n and for some properties on regularity of Padé forms, which can all be proved in one line.

Two main features of the algorithm proposed in [15] are inherited by the new variant. The first one is that it performs look-ahead steps of minimal size and the second is that it reduces to the classical Levinson [21] or Schur algorithm [22], if only regular steps of size one are performed.

This paper is an extension of [15], and we therefore want to avoid to reproduce what we proved there. Instead, we only introduce the basic notation and mention the definitions and statements we take from [15]. The paper is organized as follows. First we introduce some notation in Section 2. In Section 3 we define left and right underdetermined Padé forms. Section 4 contains the new recurrences. In Section 5, we rederive the Freund and Zha algorithms in terms of Padé approximation and show how the computational overhead of a look-ahead step can be reduced by up to a factor of two. We compare the computational work of the new algorithm and some other look-ahead algorithms available in the literature in Section 6. Finally, Section 7 contains conclusions and further developments.

2 Preliminaries and Notation

In the following,

$$\begin{aligned} \mathcal{L}_l &:= \{h \in \mathcal{L}\,;\ \mu_k = 0 \text{ if } k < l\}, \\ \mathcal{L}_m^* &:= \{h \in \mathcal{L}\,;\ \mu_k = 0 \text{ if } k > m\}, \\ \mathcal{P}_m &:= \{p \in \mathcal{L}\,;\ p \text{ polynomial of degree at most } m\} \end{aligned}$$

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

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

and $\mathcal{P}$, the set of all polynomials. The formal projection of $h \in \mathcal{L}$ into $\mathcal{L}_l \cap \mathcal{L}_m^*$ is denoted by

$$\Pi_{l:m} h(\zeta) := \sum_{j=l}^{m} \mu_j \zeta^j$$

and the mth coefficient of h is written as $\Pi_m h(\zeta) := \mu_m$. We write $h(\zeta) = O_+(\zeta^l)$ if $h(\zeta) \in \mathcal{L}_l$. With $h(\infty)$ and $h(0)$ we denote the leading coefficient of $h \in \mathcal{L}_0^*$ and $h \in \mathcal{L}_0$, respectively.

For $m \in \mathbb{Z}$ and $n \in \mathbb{N}$, where $\mathbb{Z}$ is the set of all integers and $\mathbb{N}$ is the subset of all nonnegative integers, an (m, n) *Padé form* of h is any pair $(p, q) \in$

$\mathcal{L}_m^* \times (\mathcal{P}_n \backslash \{0\})$ satisfying

$$h(\zeta)q(\zeta) - p(\zeta) = O_+(\zeta^{m+n+1}) \in \mathcal{L}_{m+n+1}. \tag{2.2}$$

The series $e \in \mathcal{L}_0$ defined implicitly by

$$h(\zeta)q(\zeta) - p(\zeta) = \zeta^{m+n+1} e(\zeta) \tag{2.3}$$

is called the *residual* of (p, q).

Padé approximations can be listed in a Padé table, where we let the m-axis point to the bottom and the n-axis point to the right. In this paper, we deal with Padé forms in the (-1)st and the 0th row of the Padé table. A key point to our derivations is the use of regular $(0, n)$ Padé forms. If we denote by $(p_n^{\nwarrow}, q_n^{\nwarrow})$ a $(-1, n-1)$ Padé form of h and by $e_n^{\nwarrow}$ its residual, then we can define a regular $(0, n)$ Padé form (p_n, q_n) in the following equivalent ways [12]:

(i) the Toeplitz matrix $\mathbf{T}_n = (\mu_{i-j})_{i,j=0}^{n-1}$ is nonsingular;
(ii) $p_n q_n^{\nwarrow} - p_n^{\nwarrow} q_n \neq 0 \ \in \mathcal{L}_{n-1}^*$;
(iii) $e_n^{\nwarrow}(0) \neq 0$ and $q_n(0) \neq 0$;
(iv) $p_n q_n^{\nwarrow} - p_n^{\nwarrow} q_n = \Delta_n^{\nwarrow} \zeta^{n-1} \neq 0$, $\Delta_n^{\nwarrow} \in \mathbb{C}$.

In order to make the notation more illustrative, we use arrows to indicate the location of neighboring Padé forms with respect to a regular $(0, n)$ Padé form of $h \in \mathcal{L}$, as we did in the above definition. Hence, we denote a $(-1, n-1)$ Padé form by $(p_n^{\nwarrow}, q_n^{\nwarrow})$, a $(-1, n)$ Padé form by $(p_n^{\uparrow}, q_n^{\uparrow})$, and a $(0, n-1)$ Padé form by $(p_n^{\leftarrow}, q_n^{\leftarrow})$. The corresponding residuals are denoted in the same way. The following picture shows the location of these Padé forms and illustrates the notation.

$$\boxed{\begin{array}{ccc} -1 & q_n^{\nwarrow} & q_n^{\uparrow} \\ 0 & q_n^{\leftarrow} & q_n \\ & n-1 & n \end{array}} \tag{2.4}$$

If (p_n, q_n) is a regular Padé form, then we call n a regular index. In this case, the four Padé forms shown in the picture can be computed by solving linear systems with coefficient matrix $\mathbf{T}_n$. They are uniquely determined up to scaling. Once we have q_n, we obtain $p_n = \Pi_{-\infty:0}(hq_n)$ and $e_n = \Pi_{n+1:\infty}(hq_n)$ from formal projections, and similar for the other Padé forms. Setting

$$q_n(\zeta) = \sum_{j=0}^{n} \rho_{j,n} \zeta^j$$

and using the analogous notation for $q_n^{\uparrow}$, $q_n^{\leftarrow}$, and $q_n^{\nwarrow}$, the coefficients of q_n and $q_n^{\uparrow}$ are determined by the well-known Yule-Walker equations

$$\mathbf{T}_n \begin{bmatrix} \rho_{1,n} \\ \vdots \\ \rho_{n,n} \end{bmatrix} = -\rho_{0,n} \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_n \end{bmatrix}, \qquad \mathbf{T}_n \begin{bmatrix} \rho_{0,n}^{\uparrow} \\ \vdots \\ \rho_{n-1,n}^{\uparrow} \end{bmatrix} = -\rho_{n,n}^{\uparrow} \begin{bmatrix} \mu_{-n} \\ \vdots \\ \mu_{-1} \end{bmatrix}$$

and the coefficients of $q_n^{\leftarrow}$ and $q_n^{\nwarrow}$ by

$$\mathbf{T}_n \begin{bmatrix} \rho_{0,n}^{\leftarrow} \\ \vdots \\ \rho_{n-1,n}^{\leftarrow} \end{bmatrix} = p_n^{\leftarrow}(\infty) \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \qquad \mathbf{T}_n \begin{bmatrix} \rho_{0,n}^{\nwarrow} \\ \vdots \\ \rho_{n-1,n}^{\nwarrow} \end{bmatrix} = e_n^{\nwarrow}(0) \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}.$$

These equations are also called *fundamental equations* [16] and their solutions are called *generators* in the context of displacement structure [20]. Since n is a regular index, we clearly have

$$\rho_{0,n} \neq 0, \quad \rho_{n,n}^{\uparrow} \neq 0, \quad p_n^{\leftarrow}(\infty) \neq 0, \quad e_n^{\nwarrow}(0) \neq 0. \tag{2.5}$$

We can therefore use the freedom we have in scaling Padé forms by setting these quantities to one and assume in the following the normalizations

$$\rho_{0,n} = 1, \quad \rho_{n,n}^{\uparrow} = 1, \quad p_n^{\leftarrow}(\infty) = 1, \quad e_n^{\nwarrow}(0) = 1. \tag{2.6}$$

Although we defined Padé forms for arbitrary $m \in \mathbb{Z}$ and $n \in \mathbb{N}$ in (2.3), we want to give the definitions of the four Padé forms in (2.4) explicitly again, because they play such a fundamental role throughout this paper:

$$\begin{aligned} hq_n - p_n &= \zeta^{n+1} e_n, & (p_n, q_n) &\in \mathcal{L}_0^* \times \mathcal{P}_n, & e_n &\in \mathcal{L}_0 \\ hq_n^{\nwarrow} - p_n^{\nwarrow} &= \zeta^{n-1} e_n^{\nwarrow}, & (p_n^{\nwarrow}, q_n^{\nwarrow}) &\in \mathcal{L}_{-1}^* \times \mathcal{P}_{n-1}, & e_n^{\nwarrow} &\in \mathcal{L}_0 \\ hq_n^{\leftarrow} - p_n^{\leftarrow} &= \zeta^{n} e_n^{\leftarrow}, & (p_n^{\leftarrow}, q_n^{\leftarrow}) &\in \mathcal{L}_0^* \times \mathcal{P}_{n-1}, & e_n^{\leftarrow} &\in \mathcal{L}_0 \\ hq_n^{\uparrow} - p_n^{\uparrow} &= \zeta^{n} e_n^{\uparrow}, & (p_n^{\uparrow}, q_n^{\uparrow}) &\in \mathcal{L}_{-1}^* \times \mathcal{P}_n, & e_n^{\uparrow} &\in \mathcal{L}_0 \end{aligned} \tag{2.7}$$

The somehow dubiously looking last three equivalent definitions (ii)–(iv) of a regular $(0, n)$ Padé form can be proved in one line by multiplying the first equation in (2.7) by $q_n^{\nwarrow}$, the second equation by q_n, and subtracting:

$$\underbrace{p_n^{\nwarrow} q_n}_{\mathcal{L}_{n-1}^*} - \underbrace{p_n q_n^{\nwarrow}}_{\mathcal{L}_{n-1}^*} = \zeta^{n-1}(\underbrace{\zeta^2 e_n q_n^{\nwarrow}}_{\mathcal{L}_2} - \underbrace{e_n^{\nwarrow} q_n}_{\mathcal{L}_0}) \in \mathcal{L}_{n-1}. \tag{2.8}$$

So, what one really has to know about Padé approximation for our purposes is that a regular index n corresponds to a nonsingular Toeplitz matrix $\mathbf{T}_n$ and one has to remember (2.7) from the definition of Padé forms. The nonsingularity of $\mathbf{T}_n$ then implies (2.5), which allows the normalization (2.6).

3 Padé forms and formally biorthogonal polynomials

As we mentioned in the introduction, the new recurrences not only use regular pairs of Padé forms but also certain underdetermined Padé forms defined below. This is motivated by the close connection between Padé forms and formally biorthogonal polynomials (FBOPs) with respect to a sesquilinear form $\langle \cdot, \cdot \rangle$ on $\mathcal{P} \times \mathcal{P}$ defined by its moments

$$\langle \zeta^i, \zeta^j \rangle := \mu_{i-j}.$$

Let h be given by (2.1) and denote by $s^\star$ the conjugated and reflected polynomial of $s \in \mathcal{P}_n$ defined as $s^\star = \zeta^n \overline{s}(\zeta^{-1})$. If $q_{n+k} \in \mathcal{P}_{n+k}$, then $\langle q_{n+k}^\star, \zeta^i \rangle = 0$ for $i = 0, \ldots, n-1$ if and only if there exists $p_{n+k} \in \mathcal{L}_k^*$ such that

$$h q_{n+k} - p_{n+k} = \zeta^{n+k+1} e_{n+k} = O_+(\zeta^{n+k+1}), \tag{3.1}$$

see [15, Lemma 7.1]. If n is a regular index and $q_{n+k}^\star$ is of full degree $n+k$, then $q_{n+k}^\star$ is called an $(n+k)$th inner left FBOP. For $k = 0$, it is an nth left FBOP [7,12,15]. Comparing (3.1) for $k = 0$ with the definition (2.7) of a $(0, n)$ Padé form of h shows the close connection to left FBOPs. From the third definition in (2.7), it follows that $\langle q_n^{\leftarrow *}, \zeta^i \rangle = 0$ for $i = 0, \ldots, n-2$. However, $q_n^{\leftarrow *}$ is an $(n-1)$st left FBOP if and only if it has full degree $n-1$, or, equivalently, if $q_n^{\leftarrow}(0) \neq 0$.

Definition 1 *If n is a regular index and $k \geq 1$, then any pair $(p_{n+k}, q_{n+k}) \in \mathcal{L}_k^* \times \mathcal{P}_{n+k}$ with $q_{n+k}(0) \neq 0$ satisfying (3.1) is called a $(0, n+k)$ left underdetermined Padé form (with respect to the regular index n), and $e_{n+k} \in \mathcal{L}_0$ is called its residual.*

Similarly it was shown in [15, Lemma 7.2], that if $q_{n+k}^{\uparrow} \in \mathcal{P}_{n+k}$, then $\langle \zeta^i, q_{n+k}^{\uparrow} \rangle = 0$ for $i = 0, \ldots, n-1$ if and only if there exists $p_{n+k}^{\uparrow} \in \mathcal{L}_{-1}^*$

such that

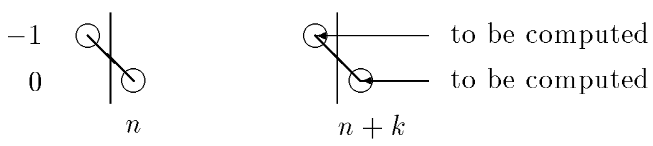
$$hq^{\uparrow}_{n+k} - p^{\uparrow}_{n+k} = \zeta^n e^{\uparrow}_{n+k} = O_+(\zeta^n). \tag{3.2}$$

Here, $q^{\uparrow}_{n+k}$ is called an $(n+k)$th inner right FBOP if n is a regular index and if $q^{\uparrow}_{n+k}$ is of full degree $n+k$. The case $k=0$ relates to the definition of a $(-1,n)$ Padé form of h, hence upper neighbors of regular Padé forms correspond to right FBOPs. It follows from the second equation in (2.7), that $\langle \zeta^i, q_n^{\nwarrow *}\rangle = 0$ for $i = 0, \ldots, n-2$. Thus $q_n^{\nwarrow}$ is an $(n-1)$st right FBOP if and only if it has full degree $n-1$.

Definition 2 *If n is a regular index and $k \geq 1$, then any pair $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k}) \in \mathcal{L}^*_{-1} \times \mathcal{P}_{n+k} \setminus \mathcal{P}_{n+k-1}$ satisfying (3.2) is called a $(-1, n+k)$ right underdetermined Padé form (with respect to the regular index n), and $e^{\uparrow}_{n+k} \in \mathcal{L}_0$ is called its residual.*

Clearly, $(0, n+k)$ left and $(-1, n+k)$ right underdetermined Padé forms exist for any $k \geq 1$. This can be seen by recognizing that the coefficient matrix of the $n \times (n+k)$ underdetermined linear system for the unknown coefficients of the denominators of the underdetermined Padé forms contains $\mathbf{T}_n$ as a submatrix. Since n is assumed to be a regular index, $\mathbf{T}_n$ is nonsingular. Thus one can choose the coefficients not belonging to this subsystem arbitrarily and then compute the unique solution of the subsystem.

Like the algorithm of [15], our new algorithm will perform regular steps identical to those of the classical Levinson or Schur algorithms whenever possible. Hence, we will consider only the look-ahead steps here. If such look-ahead steps are necessary, the new algorithm builds the same blocks as the one of [15], since it is also based on regular pairs of Padé forms. In particular, the look-ahead steps are of minimal size. However, we no longer construct two-point Padé forms to compute the regular pair, but instead use the left and right underdetermined Padé forms we computed in between. In [15], we proceeded from one regular pair to the other with the help of a suitable two-point Padé form. This can be illustrated as



where circles represent Padé forms and a line connecting two Padé forms indicates that they belong to different blocks of the Padé table. In the picture, this means that n and $n+k$ are regular indices, which is further emphasized by vertical lines. Moreover, any underdetermined Padé form in between was also computed from the regular pair corresponding to the index n. An extension of this type of algorithm to block Toeplitz matrices is given by Van Barel and Bultheel [24]. They prove that even the block algorithm is weakly stabe.

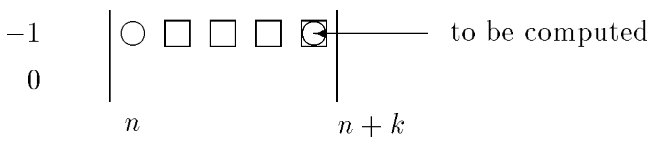
The complete block LDU decomposition of the Toeplitz matrix $\mathbf{T}$ requires the computation of residuals and numerators of Padé forms, but the computation of denominators is not necessary. Such algorithms are called *Schur-type algorithms*. *Levinson-type algorithms* compute an inverse block LDU decomposition, which contains the coefficients of denominators of Padé forms only. A block starting with the regular index n contains the coefficients of the $(-1, n)$ and the $(0, n)$ Padé forms, the $(-1, n+1), \ldots, (-1, n+k-1)$ right, and the $(0, n+1), \ldots, (0, n+k-1)$ left underdetermined Padé forms. It turns out that it pays off to compute also the $(-1, n+k-1)$ Padé form (the upper left neighbor of the regular $(0, n+k)$ Padé form) although none of the coefficients of this Padé form occur in the block decomposition of $\mathbf{T}$ or $\mathbf{T}^{-1}$. It is important to understand that the $(-1, n+k-1)$ Padé form and the $(-1, n+k-1)$ right underdetermined Padé form are different if $k > 1$.

4 Alternative recurrences

In the following, we always assume the normalization (2.6) introduced in Section 2 for regular Padé forms and $\rho_{0,n} = \rho^{\uparrow}_{n,n} = 1$, *i.e.*, the first two normalizations of (2.6), for underdetermined Padé forms.

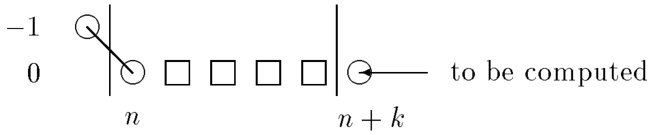
Before we state our main theorem, we would like to illustrate the recurrences by the following pictures. Here, circles represent Padé forms and squares stand for underdetermined Padé forms. The (underdetermined) Padé form distinguished by an arrow is computed from the other (underdetermined) Padé forms (or shifted copies of them) shown in the picture. Vertical lines represent the end of a look-ahead block, *i.e.*, the first column on the right of a vertical line corresponds to a regular index. In general, these lines do *not* correspond to blocks of the Padé table. In all our pictures, n and $n+k$ are assumed to be regular indices.

(4a) Compute the upper left neighbor of the regular $(0, n+k)$ Padé form, *i.e.*, the $(-1, n+k-1)$ Padé form $(p^{\nwarrow}_{n+k}, q^{\nwarrow}_{n+k})$ (represented by the circle inside the square).

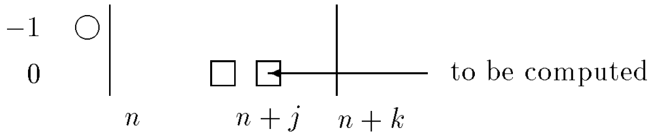


Recall that the $(-1, n+k-1)$ right underdetermined Padé form indicated by the square at the same position is different from the $(-1, n+k-1)$ Padé form we want to compute.

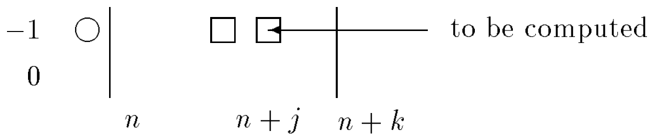
(4b) Compute the regular $(0, n+k)$ Padé form (p_{n+k}, q_{n+k}).



(4c) Compute the $(0, n+j)$ left underdetermined Padé form (p_{n+j}, q_{n+j}) from the $(0, n+j-1)$ (left underdetermined) Padé form and from the auxiliary $(-1, n-1)$ Padé form.



(4d) From the auxiliary $(-1, n-1)$ Padé form and the $(-1, n+j-1)$ (right underdetermined) Padé form compute the $(-1, n+j)$ right underdetermined Padé form $(p^{\uparrow}_{n+j}, q^{\uparrow}_{n+j})$.



The pictures clearly show that except for computing the next auxiliary upper left neighbor of a regular pair itself in (4a), the auxiliary $(-1, n-1)$ Padé form $(p^{\nwarrow}_n, q^{\nwarrow}_n)$ is used in every other recurrence of our algorithm.

In the sequel, we will use the following notation, where n still denotes a regular index:

$$e^{\uparrow}_{n+j} = \sum_{l=0}^{\infty} \varepsilon^{\uparrow}_{n+l,n+j}\zeta^{l}, \quad p_{n+j} = \sum_{l=0}^{\infty} \pi_{-j+l,n+j}\zeta^{j-l}, \quad p^{\nwarrow}_n = \sum_{l=0}^{\infty} \pi^{\nwarrow}_{l,n+j}\zeta^{-1-l}.$$

Theorem 3 *Let* (p_n, q_n), $(p^{\nwarrow}_n, q^{\nwarrow}_n)$ *be a regular pair of* $(0, n)$ *and* $(-1, n-1)$ *Padé forms of* $h \in \mathcal{L}$ *with residuals* e_n *and* $e^{\nwarrow}_n$, *and let* $(p^{\uparrow}_n, q^{\uparrow}_n)$ *be a* $(-1, n)$ *Padé form of* h *with residual* $e^{\uparrow}_n$. *Moreover, let* (p_{n+j}, q_{n+j}) *be* $(0, n+j)$ *left and* $(p^{\uparrow}_{n+j}, q^{\uparrow}_{n+j})$ *be* $(-1, n+j)$ *right underdetermined Padé forms with residuals* e_{n+j}, $e^{\uparrow}_{n+j}$, $j = 1, \ldots, k-1$, *respectively.*

(a) *If a nontrivial solution of the linear system*

$$\begin{bmatrix} \varepsilon^{\uparrow}_{n,n} & \cdots & \varepsilon^{\uparrow}_{n,n+k-1} \\ \vdots & & \vdots \\ \varepsilon^{\uparrow}_{n+k-1,n} & \cdots & \varepsilon^{\uparrow}_{n+k-1,n+k-1} \end{bmatrix} \begin{bmatrix} \theta^{\nwarrow}_0 \\ \vdots \\ \theta^{\nwarrow}_{k-1} \end{bmatrix} = \mathbf{e}_{k-1} e^{\nwarrow}_{n+k}(0) \tag{4.1}$$

exists, then $(p^{\nwarrow}_{n+k}, q^{\nwarrow}_{n+k})$ *with*

$$\begin{bmatrix} p^{\nwarrow}_{n+k} \\ q^{\nwarrow}_{n+k} \\ \zeta^{k-1} e^{\nwarrow}_{n+k} \end{bmatrix} = \sum_{j=0}^{k-1} \begin{bmatrix} p^{\uparrow}_{n+j} \\ q^{\uparrow}_{n+j} \\ e^{\uparrow}_{n+j} \end{bmatrix} \theta^{\nwarrow}_j \tag{4.2}$$

is a $(-1, n+k-1)$ *Padé form of* h *with residual* $e^{\nwarrow}_{n+k}$.

(b) *Let*

$$\vartheta_{n+k} = -e_{n+k-1}(0)/e^{\nwarrow}_n(0). \tag{4.3}$$

If a solution of

$$\begin{bmatrix} \pi_{0,n} & \cdots & \pi_{-k+1,n+k-1} \\ \vdots & & \vdots \\ \pi_{k-1,n} & \cdots & \pi_{0,n+k-1} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_{k-1} \end{bmatrix} \tag{4.4}$$

$$= - \begin{bmatrix} 0 \\ \pi_{-k+1,n+k-1} \\ \vdots \\ \pi_{-1,n+k-1} \end{bmatrix} - \begin{bmatrix} \pi^{\nwarrow}_{0,n} \\ \pi^{\nwarrow}_{1,n} \\ \vdots \\ \pi^{\nwarrow}_{k-1,n} \end{bmatrix} \vartheta_{n+k}$$

exists, then (p_{n+k}, q_{n+k}) *with*

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta e_{n+k} \end{bmatrix} = \begin{bmatrix} p_{n+k-1} \\ q_{n+k-1} \\ e_{n+k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} \zeta^{k-j} p_{n+j} \\ \zeta^{k-j} q_{n+j} \\ e_{n+j} \end{bmatrix} \theta_j + \zeta^{k+1} \begin{bmatrix} p^{\nwarrow}_n \\ q^{\nwarrow}_n \\ e^{\nwarrow}_n \end{bmatrix} \vartheta_{n+k} \tag{4.5}$$

is a $(0, n+k)$ *Padé form of* h *with* $q_{n+k}(0) = 1$ *and residual* e_{n+k}.

(c) *For* $j = 1, \ldots, k-1$, *let* $\vartheta_{n+j} = -e_{n+j-1}(0)/e_n^{\nwarrow}(0)$. *Then*

$$\begin{bmatrix} p_{n+j} \\ q_{n+j} \\ \zeta^j e_{n+j} \end{bmatrix} = \begin{bmatrix} p_{n+j-1} \\ q_{n+j-1} \\ \zeta^{j-1} e_{n+j-1} \end{bmatrix} + \begin{bmatrix} \zeta^2 p_n^{\nwarrow} \\ \zeta^2 q_n^{\nwarrow} \\ e_n^{\nwarrow} \end{bmatrix} \vartheta_{n+j} \zeta^{j-1} \tag{4.6}$$

yields a $(0, n+j)$ *left underdetermined Padé form with residual* e_{n+j}.

(d) *For* $j = 1, \ldots, k-1$, *let* $\vartheta_{n+j}^{\uparrow} = -\pi_{0,n+j-1}^{\uparrow}/\pi_{0,n}^{\nwarrow}$. *Then*

$$\begin{bmatrix} p_{n+j}^{\uparrow} \\ q_{n+j}^{\uparrow} \\ e_{n+j}^{\uparrow} \end{bmatrix} = \begin{bmatrix} p_{n+j-1}^{\uparrow} \\ q_{n+j-1}^{\uparrow} \\ e_{n+j-1}^{\uparrow} \end{bmatrix} \zeta + \begin{bmatrix} \zeta p_n^{\nwarrow} \\ \zeta q_n^{\nwarrow} \\ e_n^{\nwarrow} \end{bmatrix} \vartheta_{n+j}^{\uparrow}, \tag{4.7}$$

yields a $(-1, n+j)$ *right underdetermined Padé form with residual* $e_{n+j}^{\uparrow}$.

PROOF. First recall from (2.5) that $e_n^{\nwarrow}(0) \neq 0$ if n is a regular index. Moreover, it follows from the discussion at the end of Section 7 in [15] that in the case that we start a look-ahead step, also $\pi_{0,n}^{\nwarrow} \neq 0$. Therefore, all quotients arising in the theorem are well defined.

(a) We use (4.2) as the definition of $p_{n+k}^{\nwarrow}$ and $q_{n+k}^{\nwarrow}$. Then we have by Definition 2 and by (2.7)

$$h q_{n+k}^{\nwarrow} - p_{n+k}^{\nwarrow} = \zeta^n \sum_{j=0}^{k-1} e_{n+j}^{\uparrow} \theta_j^{\nwarrow}. \tag{4.8}$$

This series is $O_+(\zeta^{n+k-1})$ if and only if

$$\Pi_{0:k-2} \sum_{j=0}^{k-1} e_{n+j}^{\uparrow} \theta_j^{\nwarrow} = 0,$$

which is equivalent to (4.1) if one takes the normalization (2.6) into account. Moreover, $p_{n+k}^{\nwarrow} \in \mathcal{L}_{-1}^*$ since $p_{n+j}^{\uparrow} \in \mathcal{L}_{-1}^*$, and $q_{n+k}^{\nwarrow} \in \mathcal{P}_{n+k-1}$ follows from $q_{n+j} \in \mathcal{P}_{n+j}$, $j = 0, \ldots, k-1$.

(b) Again we interpret (4.5) as the definition of its left hand side. From Definition 1 we obtain

$$hq_{n+k} - p_{n+k} = \zeta^{n+k} \left(e_{n+k-1} + \zeta \sum_{j=0}^{k-1} e_{n+j}\theta_j + e_n^{\nwarrow}\vartheta_{n+k} \right). \tag{4.9}$$

This series is $O_+(\zeta^{n+k+1})$ for ϑ_{n+k} defined by (4.3). The condition $p_{n+k} \in \mathcal{L}_0^*$ is equivalent to (4.4), since $p_{n+j} \in \mathcal{L}_j^*$ and $p_n^{\nwarrow} \in \mathcal{L}_{-1}^*$. Finally, $q_{n+k} \in \mathcal{P}_{n+k}$ since $\zeta^{k-j}q_{n+j} \in \mathcal{P}_{n+k}$ and $\zeta^{k+1}q_n^{\nwarrow} \in \mathcal{P}_{n+k}$. The normalization follows from $q_{n+k-1}(0) = 1$.

(c) We have

$$hq_{n+j} - p_{n+j} = \zeta^{n+j}(e_{n+j-1} + e_n^{\nwarrow}\vartheta_{n+j}) = O_+(\zeta^{n+j+1})$$

for ϑ_{n+j} as stated in the theorem. It is easily seen that $q_{n+j} \in \mathcal{P}_{n+j}$ and, from $p_n^{\nwarrow} \in \mathcal{L}_{-1}^*$, we conclude that $p_{n+j} \in \mathcal{L}_j^*$.

(d) The approximation property is satisfied automatically:

$$hq_{n+j}^{\uparrow} - p_{n+j}^{\uparrow} = \zeta^n(\zeta e_{n+j-1}^{\uparrow} + e_n^{\nwarrow}\vartheta_{n+j}^{\uparrow}) = O_+(\zeta^n)$$

for arbitrary $\vartheta_{n+j}^{\uparrow}$. The given $\vartheta_{n+j}^{\uparrow}$ ensures $p_{n+j}^{\uparrow} \in \mathcal{L}_{-1}^*$. Finally, $q_{n+j}^{\uparrow} \in \mathcal{P}_{n+j}$, which concludes the proof. □

As we mentioned before, underdetermined Padé forms are never unique (not even up to scaling), so one has some degree of freedom in constructing them. Our choice of underdetermined polynomials leads to a block LDU factorization, where the blocks of the block diagonal matrix inherit the Toeplitz structure [15, Theorem 8.1].

We next prove a lemma concerning the length k of a look-ahead step.

Lemma 4 *Let $n = n_l$ be a regular index. Then the following two statements are equivalent:*

(a) *the index $n + k$ is a regular index,*
(b) *the coefficient matrices $\mathbf{L}^{\uparrow(l)} = (\varepsilon_{n+i,n+j}^{\uparrow})_{i,j=0}^{k-1}$ and $\mathbf{L}^{(l)} = (\pi_{i-j,n+j})_{i,j=0}^{k-1}$ in* (4.1) *and* (4.4) *are nonsingular.*

PROOF. Assume that $n + k$ is a regular index. This is equivalent to $\mathbf{T}_{n+k}$ being nonsingular. By Corollary 7.2 in [12] or [15, Section 8], the matrices $\mathbf{L}^{(l)}$ and $\mathbf{L}^{\uparrow(l)}$ are the diagonal blocks of the lower block triangular matrices

$\mathbf{L} = \mathbf{T}^H\mathbf{R}$ and $\mathbf{L}^{\uparrow} = \mathbf{T}\mathbf{R}^{\uparrow}$. Since $\mathbf{R}$ and $\mathbf{R}^{\uparrow}$ are unit upper triangular, the leading principal submatrices of $\mathbf{T}$, $\mathbf{L}$, and $\mathbf{L}^{\uparrow}$ are of same rank. Hence, $\mathbf{T}_{n+k}$ is nonsingular if and only if $\mathbf{L}^{(l)}$ and $\mathbf{L}^{\uparrow(l)}$ are nonsingular. □

The theorem shows that starting from a regular pair, one can compute subsequent underdetermined Padé forms, and from those one can obtain the next regular pair. The only recurrence missing is the one for the upper neighbor $(p_n^{\uparrow}, q_n^{\uparrow})$ of the regular Padé form (p_n, q_n). However, this is an easy task, since one can apply one of the well-known Frobenius identities, see Gragg [9, Theorem 5.2]. To give all the recurrences required by our new algorithm, we want to recall this identity from [15, Theorem 7.4]:

Theorem 5 *Let (p_n, q_n), $(p_n^{\nwarrow}, q_n^{\nwarrow})$ be a regular pair of $(0,n)$ and $(-1, n-1)$ Padé forms of $h \in \mathcal{L}$ with residuals e_n and $e_n^{\nwarrow}$, respectively. If we define*

$$\begin{bmatrix} \alpha_n \\ \beta_n \end{bmatrix} = \frac{1}{e_n^{\nwarrow}(0)} \begin{bmatrix} \pi_{0,n} \\ -\pi_{0,n}^{\nwarrow} \end{bmatrix}, \tag{4.10}$$

then

$$\begin{bmatrix} p_n^{\uparrow} \\ q_n^{\uparrow} \\ e_n^{\uparrow} \end{bmatrix} := \begin{bmatrix} \zeta p_n^{\nwarrow} & p_n \\ \zeta q_n^{\nwarrow} & q_n \\ e_n^{\nwarrow} & \zeta e_n \end{bmatrix} \begin{bmatrix} \alpha_n \\ \beta_n \end{bmatrix} \tag{4.11}$$

is a $(-1, n)$ Padé form of h with residual $e_n^{\uparrow}$.

PROOF. It was shown in [15] that [15, Theorem 7.4] is valid for $k = 0$ also. The explicit expression in (4.10) follows readily from (7.15) in [15] by exploiting that the determinant of the coefficient matrix in (7.15) is equal to $e_n^{\nwarrow}(0)$. The latter follows from (2.8). □

The following picture completes the list of recurrences used in our new algorithm:

(4e) Compute the $(-1, n)$ Padé form $(p_n^{\uparrow}, q_n^{\uparrow})$ if n is a regular index.

	Levinson algorithm	Schur algorithm
	$n = 0$	
1.	$q_0^{\uparrow} = q_0 = 1$ $\varepsilon_{0,0}^{\uparrow} = \mu_0$	$p_0^{\uparrow} = \Pi_{-\infty:-1}\, h,\ p_0 = \Pi_{-\infty:0} h$ $e_0^{\uparrow} = \Pi_{0:\infty}\, h,\ e_0 = \Pi_{1:\infty}\, h$
2.	$q_0^{\nwarrow} = 0$	$p_0^{\nwarrow} = 1,\ e_0^{\nwarrow} = -1$

WHILE $n < N$

	$k = 1$	

IF n is a column regular index

3.	$q_{n+1}^{\nwarrow} = q_n^{\uparrow}$	$p_{n+1}^{\nwarrow} = p_n^{\uparrow},\ e_{n+1}^{\nwarrow} = e_n^{\uparrow}$
4.	$\pi_{0,n}^{\uparrow} = \Pi_{-1}(hq_n^{\uparrow}),\ \varepsilon_{n,n} = \Pi_{n+1}(hq_n)$	
5.	$\gamma_0^{\uparrow(n)} = -\pi_{0,n}^{\uparrow}/\varepsilon_{n,n},\ \gamma_0^{(n)} = -\varepsilon_{n,n}/\varepsilon_{n,n}^{\uparrow}$	
6.	$q_{n+1}^{\uparrow} = \zeta q_n^{\uparrow} + q_n \gamma_0^{\uparrow(n)}$	$p_{n+1}^{\uparrow} = \zeta p_n^{\uparrow} + p_n \gamma_0^{\uparrow(n)}$ $e_{n+1}^{\uparrow} = e_n^{\uparrow} + e_n \gamma_0^{\uparrow(n)}$
7.	$q_{n+1} = \zeta q_n^{\uparrow} \gamma_0^{(n)} + q_n$	$p_{n+1} = \zeta p_n^{\uparrow} \gamma_0^{(n)} + p_n$ $e_{n+1} = \zeta^{-1}(e_n^{\uparrow} \gamma_0^{(n)} + e_n)$
8.	$\varepsilon_{n+1,n+1}^{\uparrow} = \varepsilon_{n,n}(1 - \gamma_0^{\uparrow(n)}/\gamma_0^{(n)})$	

ELSE

9.	compute required coefficients of p_n, e_n and $p_n^{\nwarrow}$, $e_n^{\nwarrow}$	

WHILE $n + k$ is not a regular index

10.	compute q_{n+k} from (4.6) compute $q_{n+k}^{\uparrow}$ from (4.7)	compute p_{n+k}, e_{n+k} from (4.6) compute $p_{n+k}^{\uparrow}$, $e_{n+k}^{\uparrow}$ from (4.7)
11.	compute required coefficients of $p_n^{\nwarrow}$, $e_n^{\nwarrow}$ and p_{n+j}, e_{n+j}, $p_{n+j}^{\uparrow}$, $e_{n+j}^{\uparrow}$, $j = 0, \ldots, k$	
	$k = k + 1$	

END WHILE ($n + k$ is not a regular index)

12.	compute regular q_{n+k} from (4.5) compute $q_{n+k}^{\nwarrow}$ from (4.2)	compute p_{n+k}, e_{n+k} from (4.5) compute $p_{n+k}^{\nwarrow}$ $e_{n+k}^{\nwarrow}$ from (4.2)
13.	compute $q_{n+k}^{\uparrow}$ from (4.11)	compute $p_{n+k}^{\uparrow}$, $e_{n+k}^{\uparrow}$ from (4.11)

END IF

	$n = n + k$	

END WHILE ($n < N$)

Table 1
Look-ahead Levinson and Schur algorithm

Note that all the desired properties of Padé forms are enforced numerically, hence the algorithm works for exact as well as for near breakdowns of the classical algorithms. For exact breakdowns, the recurrences even simplify considerably. Since this situation is more or less irrelevant in practice, we do not present these simplifications here.

In Table 1 we sketch our new look-ahead Levinson and Schur algorithm in one table in order to make the similarities clear. Step 1 is the initialization phase. Step 2 prepares for a possible look-ahead step at index 0. Steps 3–8 represent classical recurrences, Steps 9–13 look-ahead recurrences. Here, underdetermined Padé forms are computed in Steps 10–11 (Pictures (4c) and (4d)), regular pairs of Padé forms are computed in Step 12 (Pictures (4a) and (4b)). Finally, the upper neighbor of a regular Padé form is computed in Step 13 (Picture (4e)). Clearly, like for the classical recurrences (Step 5), the coefficients used from solving the linear systems (4.1) and (4.4) in Steps 10 and 12 are the same for the Levinson and for the Schur algorithm.

Detailed versions of these algorithms are given in [17]. We have implemented these and other variants from [15] in C for the particular application of solving linear systems with non-Hermitian Toeplitz coefficient matrices. Numerical experiments including comparisons with the Fortran code of the look-ahead Levinson algorithm of Chan and Hansen [3] are reported in [18]. Here, the reader can also find a discussion about look-ahead strategies and options for using the output of Levinson and Schur algorithms for solving Toeplitz systems of equations.

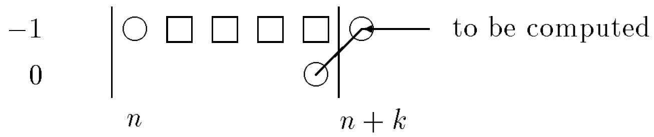
5 Related algorithms

Another approach to derive look-ahead Levinson and Schur type algorithms for computing a complete (inverse) LDU factorization of a Toeplitz matrix is by finding recurrences for formally biorthogonal polynomials. This was done by Freund and Zha [7] (Levinson algorithm) and by Freund [4] (Schur algorithm). In the notation we used within this paper, we can now interpret their recurrences in terms of Padé approximation. The statement of the following corollary is contained implicitly in [7] and [4], but we want to give an independent proof here, because it shows again the advantage of the Padé approach, where one can use the same argument to prove the Levinson and the Schur recurrences.

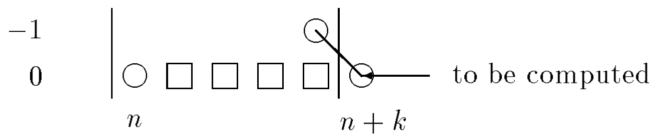
Here is an illustration of the different types of recurrences used in the algorithms [7] and [4], where the notation $\varphi_n = q_n^\uparrow$ and $\psi_n = q_n^*$ was used. As in

Section 4 we assume that n and $n+k$ are regular indices.

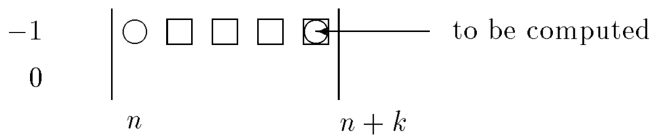
(5a) Compute the $(-1, n+k)$ Padé form $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k})$, which is the upper neighbor of the regular $(0, n+k)$ Padé form.



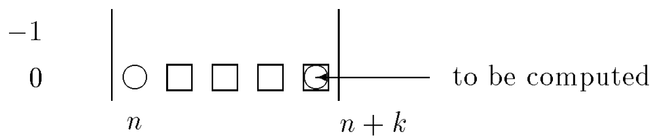
(5b) Compute the regular $(0, n+k)$ Padé form (p_{n+k}, q_{n+k}).



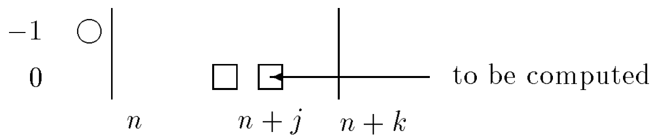
(5c) Compute the upper left neighbor of the $(0, n+k)$ Padé form, *i.e.*, the $(-1, n+k-1)$ Padé form $(p^{\nwarrow}_{n+k}, q^{\nwarrow}_{n+k})$.



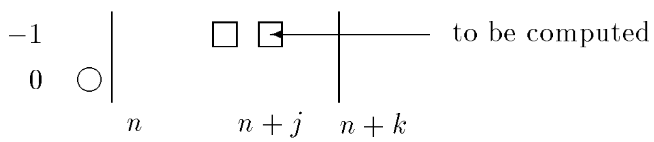
(5d) Compute the left neighbor of the $(0, n+k)$ Padé form, *i.e.*, the $(0, n+k-1)$ Padé form $(p^{\leftarrow}_{n+k}, q^{\leftarrow}_{n+k})$.



(5e) Compute the $(0, n+j)$ left underdetermined Padé form (p_{n+j}, q_{n+j}).



(5f) Compute the $(-1, n+j)$ right underdetermined Padé form $(p^{\uparrow}_{n+j}, q^{\uparrow}_{n+j})$.



Let us comment on the pictures before we give the exact recurrences in Corollary 6 below. Comparing with the pictures in Section 4, any recurrence used here also has a symmetric counterpart. However, this symmetry seems unnecessary as we have shown above. In particular, the recurrence illustrated in (5a) can be replaced by the inexpensive one (4e). Moreover (5c) can be eliminated if (5f) is replaced by (4d). We therefore renounce to give the recurrence for $q^{\leftarrow}_{n+k}$. It looks similar to (4.2). If these savings are incorporated into the algorithms [4,7], then the only difference to our new algorithm is that our recurrence to compute the next regular pair involves $q^{\nwarrow}_{n}$ and the algorithm of [7] involves $q^{\nwarrow}_{n+k}$. This should not make a big difference in the numerical behavior of the algorithms.

Note that (5e), which illustrates the recurrences for inner left FBOPs, looks identical to (4c). In fact, inner left FBOPs are computed exactly the same way as ours given in Theorem 3. For inner right FBOPs, $q^{\leftarrow}_{n}$ instead of $q^{\nwarrow}_{n}$ is used, see (4d) and (5f). This results in a block diagonal matrix of the LDU decomposition of $\mathbf{T}$, whose blocks do no longer inherit the Toeplitz structure.

We give the complete derivation only for the recurrences in pictures (5a) and (5b) in order to show how things simplify using the Padé connection. The remaining recurrences from the algorithms [4,7] have either been proved in Theorem 3 or can be eliminated. Again, we assume $q^{\uparrow}_{n}$ to be monic and $q_n(0) = 1$ for all $n = 0, 1, \ldots$.

Corollary 6 *Let the assumptions of Theorem 3 be satisfied, and assume in addition, that $n+k$ is a regular index.*

(a) *Let $\vartheta^{\uparrow}_{n+k} = -\pi^{\uparrow}_{0,n+k-1}/\pi^{\leftarrow}_{0,n+k}$. Then a unique solution of*

$$\begin{bmatrix} \varepsilon^{\uparrow}_{n,n} & \cdots & \varepsilon^{\uparrow}_{n,n+k-1} \\ \vdots & & \vdots \\ \varepsilon^{\uparrow}_{n+k-1,n} & \cdots & \varepsilon^{\uparrow}_{n+k-1,n+k-1} \end{bmatrix} \begin{bmatrix} \theta^{\uparrow}_{0} \\ \vdots \\ \theta^{\uparrow}_{k-1} \end{bmatrix} = - \begin{bmatrix} 0 \\ \varepsilon^{\uparrow}_{n,n+k-1} \\ \vdots \\ \varepsilon^{\uparrow}_{n+k-2,n+k-1} \end{bmatrix} \tag{5.1}$$

exists and $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k})$ with

$$\begin{bmatrix} p^{\uparrow}_{n+k} \\ q^{\uparrow}_{n+k} \\ \zeta^{k} e^{\uparrow}_{n+k} \end{bmatrix} = \zeta \begin{bmatrix} p^{\uparrow}_{n+k-1} \\ q^{\uparrow}_{n+k-1} \\ e^{\uparrow}_{n+k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} p^{\uparrow}_{n+j} \\ q^{\uparrow}_{n+j} \\ e^{\uparrow}_{n+j} \end{bmatrix} \theta^{\uparrow}_{j} + \begin{bmatrix} p^{\leftarrow}_{n+k} \\ q^{\leftarrow}_{n+k} \\ e^{\leftarrow}_{n+k} \end{bmatrix} \vartheta^{\uparrow}_{n+k} \tag{5.2}$$

is a $(-1, n+k)$ Padé form of h with monic $q^{\uparrow}_{n+k}$ and residual $e^{\uparrow}_{n+k}$.

(b) *Let* $\vartheta_{n+k} = -e_{n+k-1}(0)/e^{\nwarrow}_{n+k}(0)$. *Then a unique solution of*

$$\begin{bmatrix} \pi_{0,n} & \cdots & \pi_{-k+1,n+k-1} \\ \vdots & & \vdots \\ \pi_{k-1,n} & \cdots & \pi_{0,n+k-1} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_{k-1} \end{bmatrix} = - \begin{bmatrix} 0 \\ \pi_{-k+1,n+k-1} \\ \vdots \\ \pi_{-1,n+k-1} \end{bmatrix} \tag{5.3}$$

exists and (p_{n+k}, q_{n+k}) *with*

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ e_{n+k} \end{bmatrix} = \begin{bmatrix} p_{n+k-1} \\ q_{n+k-1} \\ e_{n+k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} \zeta^{k-j} p_{n+j} \\ \zeta^{k-j} q_{n+j} \\ e_{n+j} \end{bmatrix} \theta_j + \zeta \begin{bmatrix} p^{\nwarrow}_{n+k} \\ q^{\nwarrow}_{n+k} \\ e^{\nwarrow}_{n+k} \end{bmatrix} \vartheta_{n+k} \tag{5.4}$$

is a $(0, n+k)$ *Padé form of* h *with monic* $q_{n+k}(0) = 1$ *and residual* e_{n+k}.

PROOF. First observe that the coefficient matrices of both linear systems are nonsingular, if and only if $n+k$ is a regular index by Lemma 4. Moreover, if $n+k$ is a regular index, then $\varepsilon^{\nwarrow}_{n+k,n+k} \neq 0$ and $\pi^{\leftarrow}_{0,n+k} \neq 0$ by (2.5).

(a) We proceed similar to Theorem 3. From Definition 2 we obtain

$$hq^{\uparrow}_{n+k} - p^{\uparrow}_{n+k} = \zeta^n \left(\zeta e^{\uparrow}_{n+k-1} + \sum_{j=0}^{k-1} e^{\uparrow}_{n+j} \theta^{\uparrow}_j + \zeta^k e^{\leftarrow}_{n+k} \vartheta^{\uparrow}_{n+k} \right). \tag{5.5}$$

Hence, the condition $hq^{\uparrow}_{n+k} - p^{\uparrow}_{n+k} = O_+(\zeta^{n+k})$ is equivalent to (5.1). Moreover, $\zeta p^{\uparrow}_{n+k-1} + p^{\leftarrow}_{n+k} \vartheta^{\uparrow}_{n+k} \in \mathcal{L}^*_{-1}$, so that $p^{\uparrow}_{n+k} \in \mathcal{L}^*_{-1}$. The last condition, $q^{\uparrow}_{n+k} \in \mathcal{P}_{n+k}$ being monic, is obvious.

(b) Clearly, $q_{n+k} \in \mathcal{P}_{n+k}$ and $q_{n+k}(0) = 1$. We obtain from Definition 1

$$hq_{n+k} - p_{n+k} = \zeta^{n+k} \left(e_{n+k-1} + \zeta \sum_{j=0}^{k-1} e_{n+j} \theta_j + e^{\nwarrow}_{n+k} \vartheta_{n+k} \right). \tag{5.6}$$

Hence, the condition $hq_{n+k} - p_{n+k} = O_+(\zeta^{n+k+1})$ is fulfilled for ϑ_{n+k} defined as stated in the corollary. Moreover, $p_{n+k} \in \mathcal{L}^*_0$ if the coefficients θ_j solve the linear system (5.3). $\square$

Operations in a block of size $k > 1$	Levinson	Schur
inner products	$2k$	–
SAXPYs	$4k-1$	$8k-2$

Table 2
Operation counts for our new look-ahead Levinson and Schur algorithm

6 Operation counts

Recall that our new algorithm computes the same Padé forms and underdetermined Padé forms as the one proposed in [15]. Therefore, this variant of the Levinson algorithm can also be implemented by computing the same number of inner products as the classical Levinson algorithm without look-ahead, see [15, Section 8]. If we neglect computations which cost of the order $O(k^3)$ operations, where k is the (look-ahead) step size, then the only significant operations are SAXPYs and inner products. This assumption is justified as long as the look-ahead steps remain small, which is usually the case in practical applications. The computational costs of a look-ahead step in the new Levinson and Schur algorithms are given in Table 2.

In Table 3, we summarize the overhead of all the variants we proposed in this and the previous papers. For comparison, we added the overhead of other available algorithms, namely the Levinson algorithm proposed by Freund and Zha [7], the Schur algorithm of Freund [4], and the Levinson algorithm of Chan and Hansen [3]. Since all but the algorithm of Chan and Hansen [3] do not have an overhead of inner products, we list only SAXPYs. With overhead, we mean the difference of the total number of operations to construct a block of size k and the total number of operations of k steps of the corresponding classical algorithm.

The upper part of Table 3 contains algorithms which compute only regular Padé forms but no underdetermined Padé forms. Hence these algorithms do not compute a complete block LDU or inverse block LDU decomposition of $\mathbf{T}$. For Levinson type algorithms, a Toeplitz system of equations can then be solved by applying an inversion formula of Gohberg-Semencul type, see *e.g.*, [16]. However, if no complete factorization of $\mathbf{T}$ is computed, then a Schur type algorithm is only applicable for solving a Toeplitz system if the denominators of the regular Padé forms are computed also. This costs additional overhead. If one is interested only in the numerator and residual of the $(0, N)$ Padé form itself, then the computation of denominators is not necessary.

The lower part of Table 3 gives the overhead for algorithms which provide

Overhead of SAXPYs for a block of size $k > 1$	Type	Levinson	Schur
Gutknecht/Hochbruck [15]	regular	$2k-2$	$4k-4$
Huckle [19]	regular	$2k-2$	—
new algorithm	reg. + inner	$2k-1$	$4k-2$
Gutknecht/Hochbruck [15]	reg. + inner	$4k-3$	$6k-5$
Freund/Zha [7], [4]	reg. + inner	$4k$	$6k$
Chan/Hansen [3]	reg. + inner	$4k-4$	—

Table 3
Overhead for different look-ahead algorithms for solving Toeplitz systems.

a complete (inverse) block LDU decomposition of $\mathbf{T}$. For these algorithms, underdetermined Padé forms or inner FBOPs are computed also. Our new variant turns out to be the cheapest method known today. In particular, its Levinson form has only roughly half the overhead of other methods that also produce the full inverse LDU decomposition of $\mathbf{T}$.

As in the variants in [15], overhead occurs only in look-ahead steps. In a regular step ($k = 1$), we do not have to compute $q_n^{\nwarrow}$, $p_n^{\nwarrow}$, and $e_n^{\nwarrow}$, since these are just rescaled versions of $q_{n-1}^{\uparrow}$, $p_{n-1}^{\uparrow}$, and $e_{n-1}^{\uparrow}$. Clearly, this scaling is done only implicitly.

Note that the overhead of a look-ahead step in the new Schur algorithm is twice as high as that of the Levinson algorithm. This is due to the fact that numerators and residuals of all underdetermined Padé forms have to be computed, while the Levinson algorithm computes only denominators. However, recall that for the Schur algorithm proposed in [15], the same argument does not apply, since even if the complete factorization is computed, this factorization contains only numerators but not residuals of $(0, n+j)$ left underdetermined Padé forms and residuals but not numerators of $(-1, n+j)$ right underdetermined Padé forms [12, Theorem 7.1]. Hence here, the overhead for computing underdetermined Padé forms is the same as in the Levinson algorithm. Additional overhead comes only from computing the regular pair.

7 Conclusions and further developments

In this paper, we have shown how regular pairs and suitably defined underdetermined Padé forms can be used to derive efficient algorithms to compute certain Padé forms in adjacent rows of the Padé table. This approach is also applicable to other algorithms, such as the look-ahead Hankel solvers described in [2,11] or the look-ahead Lanczos algorithm in its three-term [5] or its coupled two-term version [6]. These algorithms are based on recurrences along one diagonal or along two adjacent diagonals in the Padé table. Moreover, it seems possible to extend our new algorithm to block Toeplitz matrices, similar to the extensions [23,24].

While for Toeplitz and Hankel solvers algorithms which contain as its main computational tool polynomial multiplications seem fairly attractive, in particular due to the possibility to make them superfast, this situation is totally different for the Lanczos or the isometric Arnoldi algorithm [10]. Here, performing polynomial multiplications would mean to perform matrix-vector multiplications. Since matrix-vector multiplications usually dominate the computational cost, this is overhead one definitely wants to save. Hence, for this application, the only option is to take an approach similar to the one presented here and incorporate inner formally orthogonal polynomials into the computation. Substantial savings in the algorithms of [5,6] can be achieved by using regular, row-regular or column-regular pairs in these algorithms. For example, using regular pairs in the three-term version of the look-ahead Lanczos algorithm avoids to orthogonalize inner vectors against the complete previous block. Moreover, regular vectors need then only be orthogonalized against the last block and one further vector. For the Levinson type (block) Hankel solvers such a simplification was exploited in [8,23] already without using the relation to Padé approximation. For details we refer to [17].

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