A uniform approach for the fast computation of Matrix-type Padé approximants

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Abstract

Recently, a uniform approach was given [5] for different concepts of matrix-type Padé approximants, such as descriptions of vector and matrix Padé approximants along with generalizations of simultaneous and Hermite Padé approximants. The considerations in this paper are based on this generalized form of the classical scalar Hermite Padé approximation problem, *power Hermite Padé approximation*. In particular we study the problem of computing these new approximants.

A recurrence relation is presented for the computation of a basis for the corresponding linear solution space of these approximants. This recurrence also provides bases for particular subproblems. This generalizes previous work by Van Barel and Bultheel and, in a more general form, by Beckermann. The computation of the bases has complexity $\mathcal{O}(\sigma^2)$ where σ is the order of the desired approximant, and requires no conditions on the input data. A second algorithm using the same recurrence relation along with divide-and-conquer methods is also presented. When the coefficient field allows for fast polynomial multiplication this second algorithm computes a basis in the superfast complexity $\mathcal{O}(\sigma \log^2 \sigma)$. In both cases the algorithms are reliable in exact arithmetic, that is, they never break down, and the complexity depends neither on any normality assumptions nor on the singular structure of the corresponding solution table. As a further application, our methods result in fast (and superfast), reliable algorithms for the inversion of striped Hankel, layered Hankel and (rectangular) block-Hankel matrices.

Key words: Vector Padé approximant, Hermite Padé approximant, simultaneous Padé approximant, matrix Padé approximant, Hankel matrices.

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1 Introduction

Let $\mathbf{F} = (f_1, \ldots, f_m)^T$ (with $m \geq 2$) be an m-tuple of formal power series with coefficients from a field $\mathbb{K}$ (typically a subfield of either the real or complex numbers) and $\mathbf{n} = (n_1, \ldots, n_m)$ an m-tuple of integers, $n_l \geq -1$. A *Hermite Padé approximant* for $\mathbf{F}$ of type $\mathbf{n}$ is a nontrivial tuple $\mathbf{P} = (P_1, \ldots, P_m)$ of polynomials P_l over $\mathbb{K}$ having degrees bounded by the n_l such that

$$\mathbf{P}(z) \cdot \mathbf{F}(z) = P_1(z) f_1(z) + \ldots + P_m(z) f_m(z) = c_N z^N + c_{N+1} z^{N+1} + \ldots, \qquad (1)$$

with $N = n_1 + \ldots + n_m + m - 1$.

The *Hermite Padé approximation problem* was introduced in 1873 by Hermite and has been widely studied by several authors (for a bibliography, see, e.g. [2, 3, 4] or [25]). Note that when $m = 2$, $\mathbf{F} = (f, -1)^T$ equation (1) is the same as

$$P_1(z) f(z) - P_2(z) = O(z^{n_1+n_2+1})$$

and hence as a special case we have the classical Padé approximation problem for a power series f. Hermite Padé approximation also includes other classical approximation problems such as algebraic approximants ($\mathbf{F} = (1, f, f^2, \ldots, f^{m-1})^T$) (e.g. [23] for the special case $m = 2$) and G^3J approximants ($m = 3$, $\mathbf{F} = (f', f, 1)^T$). We refer the reader to [1, pp.32-40] for additional examples. More generally, there is the *M-Padé approximation problem* which requires that $\mathbf{P} \cdot \mathbf{F}$ vanishes at a given set of knots $z_0, z_1, \ldots, z_{N-1}$, counting multiplicities ([2, 3, 4], [20], [21]). The case where all the z_i are equal to 0 is just the Hermite Padé problem.

Hermite also defined a second type of approximant to a vector of power series, the so-called *simultaneous Padé approximants* and used them in his proof of the transcendence of e. Close connections between these two approximation problems have been pointed out in [7, 14, 16, 17, 21].

In recent years, several vector and matrix generalizations of these approximation problems have been given (see Section 2). The aim of this paper is to study a uniform approach not only to Hermite Padé and simultaneous Padé approximants but also to their matrix-type generalizations. To this end, we consider the following generalized scalar Hermite Padé approximation problem [5]:

Definition 1.1. (PHPA) *Let $\sigma \geq 0$, $s > 0$, $n_1, \ldots, n_m$ be integers, $n_l \geq -1$ and $\mathbf{n} = (n_1, \ldots, n_m)$. Then a* Power Hermite Padé approximant *(PHPA) $\mathbf{P} = (P_1, \ldots, P_m)$ of type $(\mathbf{n}, \sigma, s)$ consists of scalar polynomials P_l having degrees bounded by the n_l with*

$$R(z) = \mathbf{P}(z^s) \cdot \mathbf{F}(z) = P_1(z^s) f_1(z) + \ldots + P_m(z^s) f_m(z) = c_\sigma z^\sigma + c_{\sigma+1} z^{\sigma+1} + \ldots, \qquad (2)$$

that is, has order σ. The power series R will be referred to as the s-residual. □

The power s appearing in Definition 1.1 provides a method of converting a vector problem into a scalar problem (see Section 2). By defining these approximants in a similar way to Hermite Padé approximants we can borrow from the (successful) computational techniques for the Hermite Padé problem used in [2, 4, 25]. Of course the classical Hermite Padé approximation problem is included by setting $s = 1$ and $\sigma = \|\mathbf{n}\| - 1$, where the norm of multi-indices $\mathbf{n} = (n_1, \ldots, n_m) \in (\mathbb{N}_0 \cup \{-1\})^m$ is defined by $\|\mathbf{n}\| := (n_1 + 1) + \ldots + (n_m + 1)$. Note that, by equating coefficients, equation (2) results in a system of homogeneous linear equations. By comparing the number of unknowns to equations one can conclude that there exist at least $\|\mathbf{n}\| - \sigma$ PHPA's of type $(\mathbf{n}, \sigma, s)$ which are linearly independent over $\mathbb{K}$.

The paper is organized as follows: Section 2 gives examples of matrix-type generalizations of existing approximation problems. These are shown to be special cases of the PHPA problem for various values of s and σ. In Section 3 we provide a recursive algorithm to efficiently and reliably solve the PHPA problem in exact arithmetic. Some interesting properties of our algorithm along with a cost analysis is given in Section 4. It is shown that the algorithm is at least as fast or faster than existing methods for special cases. Thus our results provide a uniform method of computing matrix-type generalizations of Padé approximation problems. Section 5 gives an example of the use of this algorithm in the context of square-matrix Padé approximants. Section 6 considers a modification of our algorithm that combines divide-and-conquer techniques along with the recurrence relation of Section 3. When the field $\mathbb{K}$ allows fast polynomial multiplication the resulting new algorithm solves the PHPA problem with superfast complexity. Finally, the paper closes with a discussion of a number of research directions that follow from our work.

For purposes of presentation, we adopt the following notations. Let $\mathcal{S}$ be a space with scalars from $\mathbb{K}$, for instance $\mathcal{S} = \mathbb{K}^{(p \times q)}$, the space of $p \times q$ matrices over $\mathbb{K}$. Then $\mathcal{S}[z]$ will denote the set of polynomials in z with coefficients from $\mathcal{S}$ while $\mathcal{S}[[z]]$ represents the set of formal power series in z with coefficients from $\mathcal{S}$. Multi-indices and PHPA's will be denoted in bold face letters; they are both $(1 \times m)$ row vectors. Also, throughout this paper the parameter s and the multi-index $\mathbf{n}$ will be fixed. The algorithm of Section 3 follows along an m-dimensional 'diagonal' path $(\mathbf{n}(\delta))_{\delta \in \mathbb{Z}}$ induced by $\mathbf{n}$ which is defined as follows:

$$\delta \in \mathbb{Z}, \mathbf{n} = (n_1, \ldots, n_m) : \mathbf{n}(\delta) = (n_1', \ldots, n_m') \text{ with } n_l' = \max\{-1, n_l + \delta\}. \qquad (3)$$

This notion allows us to discuss not only one approximation problem corresponding to $\mathbf{n} = \mathbf{n}(0)$, but also simultaneously all subproblems associated with $\mathbf{n}(\delta)$, $\delta < 0$ (cf. Table 3). Finally, the set of all PHPA's of type $(\mathbf{n}(\delta), \sigma, s)$ is denoted as $\mathcal{L}_\delta^\sigma$; it is a finite-dimensional space over $\mathbb{K}$.

Parallel to and independently of [5] and our present work, another uniforming approach has been proposed in [26] by Van Barel and Bultheel based on the concept of vector M-Padé approximation. Their approach does not reduce to a simple scalar concept as does the notion of our PHPA's. However, their approach does have the advantage of handling matrix rational interpolation and so it can be seen complementary to this paper.

2 Matrix-type Padé approximants as special PHPA's

In this section we give examples of a number of matrix-type generalizations of classical Padé approximation problems. Let A be a $p \times q$ matrix of power series over $\mathbb{K}$ and suppose $r \in \mathbb{N}$ and $M, N \in \mathbb{N}_0$.

Example 2.1. (Right-hand square and rectangular Matrix-Padé Forms) *Find $P \in \mathbb{K}^{(p\times r)}[z]$, $Q \in \mathbb{K}^{(q\times r)}[z]$, with* deg $P \leq M$, deg $Q \leq N$ *and the columns of Q being linearly independent over $\mathbb{K}$ such that*

$$A(z) \cdot Q(z) - P(z) = z^{M+N+1} \cdot R(z),$$

with $R \in \mathbb{K}^{(p\times r)}[[z]]$. □

Example 2.2. (Left-hand square and rectangular Matrix-Padé Forms) *Find $P \in \mathbb{K}^{(r\times q)}[z]$, $Q \in \mathbb{K}^{(r\times p)}[z]$, with* deg $P \leq M$, deg $Q \leq N$ *and the rows of Q being linearly independent over $\mathbb{K}$ such that*

$$Q(z) \cdot A(z) - P(z) = z^{M+N+1} \cdot R(z),$$

with $R \in \mathbb{K}^{(r\times q)}[[z]]$. □

When $p = q = r = 1$ this is the classical scalar Padé approximation problem. When $p = q = r > 1$ these are square right-hand or left-hand matrix Padé approximants [19]. In the rectangular ($p \neq q$) case, two natural matrix Padé approximations occur when either $p = r$ or $q = r$. Both of these rectangular-matrix types of Padé forms are used, for example, to compute the inverse of matrices partitioned into a rectangular-block Hankel structure [18].

We remark that, in the examples where $Q(z)$ is square, it is of special interest to determine those cases where we can form a Padé fraction $P(z) \cdot Q(z)^{-1}$ or $Q(z)^{-1} \cdot P(z)$ as an approximant to $A(z)$. In both cases we are therefore interested in necessary and sufficient conditions under which $Q(z)$ is non-singular.

Motivated by the well-known connections between left-hand and right-hand square matrix Padé forms and by inversion formulas of block Hankel-like matrices, one of the authors [17] introduced for $p, \mu \in \mathbb{N}$ and $\rho_0, \ldots, \rho_\mu \geq 0$, $\rho = \rho_0 + \ldots + \rho_\mu$, $A_0, \ldots, A_\mu \in \mathbb{K}^{p \times p}[[z]]$:

Example 2.3. (Matrix Hermite Padé Form) *Find polynomials* $P_0, \ldots, P_\mu \in \mathbb{K}^{p \times p}[z]$ *with* $\deg P_l \leq \rho_l - 1$, $0 \leq l \leq \mu$ *and*

$$A_0(z)P_0(z) + \ldots + A_\mu(z)P_\mu(z) = z^{\rho-1} \cdot R(z),$$

$R \in \mathbb{K}^{p \times p}[[z]]$ *such that the matrix* $[P_0, \ldots, P_\mu] \in \mathbb{K}^{p \times (\mu+1)p}[z]$ *has full rank over* $\mathbb{K}$. □

Example 2.4. (Matrix Simultaneous Padé Form) *Find polynomials* $Q_0, \ldots, Q_\mu \in \mathbb{K}^{p \times p}[z]$ *with* $\deg Q_l \leq \rho - \rho_l$, $0 \leq l \leq \mu$ *and*

$$Q_0(z)A_l(z) - Q_l(z)A_0(z) = z^{\rho+1} \cdot R_l(z),$$

$1 \leq l \leq \mu$, $R_l \in \mathbb{K}^{p \times p}[[z]]$ *such that the matrix* $[Q_0, \ldots, Q_\mu] \in \mathbb{K}^{p \times (\mu+1)p}[z]$ *has full rank over* $\mathbb{K}$. □

Beside the classical scalar simultaneous Padé approximants ($p = 1$, $A_0(z) = 1$), Example 2.4 also includes the *simultaneous partial Padé approximation problem* where we have prescribed poles and zeros for the approximants [8]. Following [22], the question of irreducible Hermite Padé forms is of special interest, i.e., we also require that $[P_0(0), \ldots, P_\mu(0)] \in \mathbb{K}^{p \times (\mu+1)p}$ is different from zero (or moreover has full rank over $\mathbb{K}$). Similarly, in Example 2.4 we are interested in approximants where $Q_0(0)$ is a non-singular matrix.

We remark that the order conditions in Examples 2.1 to 2.4 are all such that at least one solution exists for each approximation problem. In addition, the so-called *Weak Matrix Hermite Padé Form* and *Weak Matrix Simultaneous Padé Form* are connected to Examples 2.3 and 2.4 (see [17]). In this case the order conditions are weakened to allow for more linearly independent solutions. Other examples of matrix-type generalizations of Padé approximants include Hermite Padé Systems [11] and Simultaneous Padé Systems [12], [17]. These, however, only exist in certain cases.

Note that the Matrix Simultaneous Padé Form is closely connected to a rectangular Matrix Hermite Padé Form if the interpolation conditions are written as follows:

$$\begin{bmatrix} A_1^T(z) \\ A_2^T(z) \\ A_3^T(z) \\ \vdots \\ A_\mu^T(z) \end{bmatrix} \cdot Q_0^T(z) + \begin{bmatrix} -A_0^T(z) \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \cdot Q_1^T(z) + \ldots + \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ -A_0^T(z) \end{bmatrix} \cdot Q_\mu^T(z) = z^{\rho+1} \cdot \begin{bmatrix} R_1^T(z) \\ R_2^T(z) \\ R_3^T(z) \\ \vdots \\ R_\mu^T(z) \end{bmatrix}$$

All examples given here are special cases of so-called Vector Hermite Padé approximants.

Example 2.5. **(Vector Hermite Padé approximant)** *Let* $m, s, \tau \in \mathbb{N}_0$, $m, s \geq 2$, $G_1, \ldots, G_m \in \mathbb{K}^{s\times 1}[[z]]$ *and let* $\mathbf{n}$ *be a multi-index. Find linearly independent polynomial tuples* $(P_1, \ldots, P_m)$, $P_l \in \mathbb{K}[z]$ *with* $\deg P_l \leq n_l$, $1 \leq l \leq m$ *such that*

$$G_1(z)P_1(z) + \ldots + G_m(z)P_m(z) = z^\tau \cdot R(z),$$

with $R \in \mathbb{K}^{s\times 1}[[z]]$. □

By setting

$$\text{for } 1 \leq l \leq m\text{: } f_l(z) = (1, z, z^2, \ldots, z^{s-1}) \cdot G_l(z^s), \tag{4}$$

we see that computing Vector Hermite Padé approximants of type $(\mathbf{n}, \tau)$ and dimension s is equivalent to the determination of PHPA's of type $(\mathbf{n}, \tau s, s)$, i.e. of the solution set $\mathcal{L}_0^{\tau s}$. Indeed the above technique of converting a vector problem to a scalar problem via the raising of z to the s-th power provides the motivation for our Definition 1.1.

In Table 1, we have listed the particular choices of $m, \mathbf{n}, s, \sigma, \mathbf{F}$ with respect to Examples 2.1, 2.2 and 2.3. Instead of 2.4, we consider the special case of scalar simultaneous Padé approximation.

Example	m	s	σ	$\mathbf{n}$, $\mathbf{F}$	No. sol.
classical Hermite Padé	m	1	$\|\mathbf{n}\| - 1$	$(n_1, \ldots, n_m)$, $\mathbf{F}^T(z) = (f_1(z), .., f_m(z))$	1
2.1	$p+q$	p	$p(M+N+1)$	$(M, .., M, N, .., N)$, $\mathbf{F}^T(z) = (1, z, .., z^{p-1}) \cdot \big(\mathbf{I}, -A(z^p)\big)$	r
2.2	$p+q$	q	$q(M+N+1)$	$(M, .., M, N, .., N)$, $\mathbf{F}(z) = \begin{pmatrix} \mathbf{I} \\ -A(z^q) \end{pmatrix} \cdot (1, z, .., z^{q-1})^T$	r
2.3	$p(\mu+1)$	p	$p(\rho-1)$	$(\rho_0 - 1, ., \rho_0 - 1, .., \rho_\mu - 1, ., \rho_\mu - 1)$, $\mathbf{F}^T(z) = (1, z, .., z^{p-1})\cdot$ $\big(A_0(z^p), .., A_\mu(z^p)\big)$	p
2.4 with $p=1, A_0 = 1$	$\mu+1$	μ	$\mu(\rho+1)$	$(\rho - \rho_0, .., \rho - \rho_\mu)$, $f_1(z) = -\sum_{1\leq j\leq \mu} z^{j-1} A_j(z^\mu)$ $j \geq 1 : f_{j+1}(z) = z^{j-1}$	1

TABLE 1: Specification of the PHPA parameters used in (2) for some Matrix-type Padé Approximation problems. The integer in the last column denotes the number of PHPA solutions required to construct the corresponding Matrix-type Padé approximant.

3 Recursive computation of PHPA bases

In this section, we construct systems of m PHPA's by recurrence on σ. This allows us to describe all the PHPA's of type $(\mathbf{n}(\delta), \sigma, s)$, $\delta \leq 0$, when a fixed s, $\mathbf{F}$ and $\mathbf{n}$ are given. Therefore we not only solve the Hermite Padé approximation problem of type $\mathbf{n}$ or the corresponding matrix-type Padé approximation problem (see Section 2) but also all subproblems of type $\mathbf{n}(\delta)$, $\delta \leq 0$ (cf. Eqn. (3)) belonging to a 'diagonal path' in the solution table. The recurrence formula and the resulting algorithm do not require any assumptions on the input data $\mathbf{F}$. Moreover, the algorithm is fast, i.e. it always has a complexity of $\mathcal{O}(\|\mathbf{n}\|^2)$ arithmetic operations whereas the classical Gaussian algorithm, applied on the corresponding system of linear equations, has complexity $\mathcal{O}(\|\mathbf{n}\|^3)$ because it does not take into account the special structure of the matrix of coefficients. Finally, our method is also reliable which in this context means that it also recognizes insoluble problems or gives representations if the solution sets of type $\mathbf{n}(\delta)$, $\delta < 0$ are multi-dimensional (assuming that exact arithmetic is available). We remark that our algorithm does not consider the case of floating point arithmetic, and hence does not consider the issue of numerical stability in the presence of roundoff errors

Several fast algorithms for special cases of PHPA's are well-known but most of them require a normal or perfect solution table (i.e. PHPA's of different type are distinct). As far as we know, only the methods proposed in [19] for square matrix Padé approximation and the Jacobi-Perron continued fraction algorithm of [6] for simultaneous Padé approximation and [2, 4, 11, 12, 25] for scalar Hermite Padé approximation are also reliable. All of them still require slight assumptions on the input data ($A(0)$ regular, $\mathbf{F}(0)$ nontrivial), moreover, the algorithms of [11], [12], [19] might reach a complexity $\mathcal{O}(\|\mathbf{n}\|^3)$ if none of the subproblems of type $\mathbf{n}(\delta)$, $\delta < 0$ has a unique solution.

For the special case $s = 1$ (i.e. scalar Hermite Padé approximation), the recurrence formula of our new algorithm is similar to that used in [2, 4, 25]. The *fast Gaussian algorithm* [2, Sec.5] is motivated by the close connections to the factorization of the corresponding matrix of coefficients via the Gaussian algorithm with partial pivoting, a 'special rule' reduces the complexity to $\mathcal{O}(\|\mathbf{n}\|^2)$. It provides solutions to all subproblems on the 'diagonal path' $(\mathbf{n}(\delta))_{\delta\leq 0}$. The methods of [2, 4] both are developed for the more general M-Padé approximation problem (arbitrary interpolation knots), moreover, by the algorithm given in [4] we can compute solutions by recurrence on 'arbitrary paths' or 'staircases' $(\mathbf{n}_k)$ where the multi-index $\mathbf{n}_{k+1}$ differs from $\mathbf{n}_k$ by increasing one component (also the decreasing of a second component is allowed). Parallel to [2, 4], Van Barel and Bultheel proposed a fast, reliable method for computing Hermite Padé approximants on 'diagonal paths' [25]. Their version is similar to [2] but notationally less complicated. The ideas developed in [26] for a recursive computation of vector M-Padé approximants have close connections to [4, 25]. The authors propose three alternative 'basic steps' which includes considerable freedom in solving certain subproblems.

There seems to be no connection between the methods described above and the reliable Jacobi-Perron continued fraction algorithm of [6] for simultaneous Padé approximation. For this approximation problem, using our formalism we obtain a more compact method with at most the same complexity, in addition we get more information about singular cases.

Before describing bases for PHPA solution sets let us introduce the following:

Definition 3.1. (defect, order) *The* defect *of a* $\mathbf{P} = (P_1, \ldots, P_m) \in \mathbb{K}^m[z]$ *(with respect to the fixed multi-index* $\mathbf{n} = (n_1, \ldots, n_m)$*) is*

$$\text{dct } \mathbf{P} := \min_l \{n_l + 1 - \deg P_l\}$$

where the zero polynomial has degree $-\infty$. *The* order *of* $\mathbf{P}$ *(with respect to* $s \in \mathbb{N}$ *and* $\mathbf{F}$*) is defined by*

$$\text{ord } \mathbf{P} := \sup\{\sigma \in \mathbb{N}_0 : \mathbf{P}(z^s) \cdot \mathbf{F}(z) = z^\sigma \cdot R(z) \textit{ with } R \in \mathbb{K}[[z]]\}.$$

□

The definition of the defect is a natural extension of that found in the case of the M-Padé problem (cf., [3, 4]) and its special case of rational interpolation (some authors use a slightly different definition). The defect is also closely connected to the τ-degree of [25].

Using Definition 3.1, we get an equivalent characterization for PHPA solution sets:

$$\text{For } \sigma \in \mathbb{N}_0,\ \delta \in \mathbb{Z} \cup \{+\infty\}\text{: } \mathcal{L}_\delta^\sigma = \{\mathbf{P} \in \mathbb{K}^m[z] : dct\, \mathbf{P} > -\delta, ord\, \mathbf{P} \geq \sigma\}. \quad (5)$$

Now we are able to describe so-called σ-bases of PHPA's.

Definition 3.2. (σ-bases) *Let* $\sigma \in \mathbb{N}_0$. *The system* $\mathbf{P}_1, \ldots, \mathbf{P}_m \in \mathbb{K}^m[z]$ *is called a* σ-basis *if and only if:*

(a) $\mathbf{P}_1, \ldots, \mathbf{P}_m \in \mathcal{L}_{+\infty}^\sigma$, *i.e.* ord $\mathbf{P}_l \geq \sigma$

(b) *For each* $\delta \in \mathbb{Z} \cup \{+\infty\}$ *and for each* $\mathbf{Q} \in \mathcal{L}_\delta^\sigma$ *there exists one and only one tuple of polynomials* $(\alpha_1, \ldots, \alpha_m)$, deg $\alpha_l <$ dct $\mathbf{P}_l + \delta$ *such that* $\mathbf{Q} = \alpha_1 \cdot \mathbf{P}_1 + \ldots + \alpha_m \cdot \mathbf{P}_m$. □

Note that, as a consequence of Definition 3.2, a σ-basis $\mathbf{P}_1, \ldots, \mathbf{P}_m$ must be linearly independent with respect to polynomial coefficients. Moreover we have

$$\mathcal{L}_\delta^\sigma = \text{span}\{z^j \cdot \mathbf{P}_l : 1 \leq l \leq m, 0 \leq j < dct\, \mathbf{P}_l + \delta\} \quad (6)$$

$$\dim \mathcal{L}_\delta^\sigma = \max\{dct\, \mathbf{P}_1 + \delta, 0\} + \ldots + \max\{dct\, \mathbf{P}_m + \delta, 0\}. \quad (7)$$

The existence of σ-bases for the case $s=1$ was given in [2, 3, 4, 25] and for the case $s>1$ in [5]. Before giving an algorithm for their computation, let us state some simple rules for the defect and order of linear combinations of PHPA's.

Lemma 3.3 *For* $\mathbf{P},\mathbf{Q}\in \mathbb{K}^m[z]$, $c\in\mathbb{K}\setminus\{0\}$*:*

$$\text{dct } (c\cdot\mathbf{P}) = \text{dct } \mathbf{P}\ ,\ \text{dct } (\mathbf{P}+\mathbf{Q}) \geq \min\{\text{dct } \mathbf{P},\text{dct } \mathbf{Q}\}\ ,\ \text{dct } (z\cdot\mathbf{P}) = \text{dct } \mathbf{P}-1\ , \quad (8)$$

$$\text{ord } (c\cdot\mathbf{P}) = \text{ord } \mathbf{P}\ ,\ \text{ord } (\mathbf{P}+\mathbf{Q}) \geq \min\{\text{ord } \mathbf{P},\text{ord } \mathbf{Q}\}\ ,\ \text{ord } (z\cdot\mathbf{P}) = \text{ord } \mathbf{P}+s\ . \quad (9)$$

Proof: Left to the reader. □

From the characterization (5) it is clear that $\mathcal{L}^\sigma_\delta\subset\mathcal{L}^\sigma_{\delta+1}$ and $\mathcal{L}^{\sigma+1}_\delta\subset\mathcal{L}^\sigma_\delta$. In addition, if $\mathbf{P}\in\mathcal{L}^\sigma_\delta\setminus\mathcal{L}^{\sigma+1}_\delta$, i.e. *ord* $\mathbf{P}=\sigma$, then from (8), (9) it is easy to see that for each $\mathbf{Q}\in\mathcal{L}^\sigma_\delta$ there exists a $c\in\mathbb{K}$ such that $\mathbf{Q}-c\cdot\mathbf{P}\in\mathcal{L}^{\sigma+1}_\delta$. This proves the statement

$$\mathcal{L}^{\sigma+1}_\delta\subset\mathcal{L}^\sigma_\delta\ ,\ \dim\,\mathcal{L}^{\sigma+1}_\delta\geq\ \dim\,\mathcal{L}^\sigma_\delta-1 \quad (10)$$

and already gives an idea about the computation of σ-bases by recurrence on the order as proposed in the procedure FPHPS (*'Fast Power Hermite Padé Solver'*) below. We show in Theorem 3.4 that this method is both correct and produces the desired σ-bases.

ALGORITHM FPHPS

INPUT: $m\geq 2$, $s\in\mathbb{N}$, $\mathbf{F}=(f_1,\ldots f_m)^T$, multi-index $\mathbf{n}=(n_1,\ldots,n_m)$

INITIALIZATION: Let for $\sigma=0$, $l=1,\ldots,m$:
$d_{l,0}=n_l$, $\mathbf{P}_{l,0}=(0,..,0,1,0,..,0)$ (lth unit vector)

RECURSIVE STEP: For $\sigma=0,1,2,\ldots$:
Let for $l=1,\ldots,m$: $c_{l,\sigma}=z^{-\sigma}\cdot\mathbf{P}_{l,\sigma}(z^s)\cdot\mathbf{F}(z)\mid_{z=0}$ and $\Lambda_\sigma=\{l: c_{l,\sigma}\neq 0\}$

CASE $\Lambda_\sigma=\{\}$, then for $l=1,\ldots,m$:
$\mathbf{P}_{l,\sigma+1}=\mathbf{P}_{l,\sigma}$, $d_{l,\sigma+1}=d_{l,\sigma}$

CASE $\Lambda_\sigma\neq\{\}$, then let $\pi=\pi_\sigma\in\Lambda_\sigma$ be defined by
$d_{\pi,\sigma}=\max\{d_{l,\sigma}: l\in\Lambda_\sigma\}$
and compute for $l=1,\ldots,m$:
$l\in\Lambda_\sigma, l\neq\pi$: $\mathbf{P}_{l,\sigma+1}=\mathbf{P}_{l,\sigma}-\frac{c_{l,\sigma}}{c_{\pi,\sigma}}\cdot\mathbf{P}_{\pi,\sigma}$, $d_{l,\sigma+1}=d_{l,\sigma}$
$l\notin\Lambda_\sigma$: $\mathbf{P}_{l,\sigma+1}=\mathbf{P}_{l,\sigma}$, $d_{l,\sigma+1}=d_{l,\sigma}$
$l=\pi$: $\mathbf{P}_{\pi,\sigma+1}=z\cdot\mathbf{P}_{\pi,\sigma}$, $d_{\pi,\sigma+1}=d_{\pi,\sigma}-1$

OUTPUT: For $\sigma=0,1,2,\ldots$:
σ-bases $\mathbf{P}_{1,\sigma},\ldots,\mathbf{P}_{m,\sigma}$ with *dct* $\mathbf{P}_{l,\sigma}=d_{l,\sigma}+1$, $l=1,\ldots,m$, i.e.
for all δ: $\mathcal{L}^\sigma_\delta=\{\alpha_1\cdot\mathbf{P}_{1,\sigma}+\ldots+\alpha_m\cdot\mathbf{P}_{m,\sigma}:\ \textit{deg}\ \alpha_l\leq d_{l,\sigma}+\delta\}$.

Theorem 3.4. (Feasibility of method FPHPS) *Method FPHPS is well-defined and gives the specified results.*

Proof: We show the assertion by induction on σ for a fixed δ.

The case $\sigma = 0$ follows immediately from the definition of $\mathcal{L}_\delta^0$. Hence suppose $\sigma \geq 0$ and that the algorithm is correct for σ. We will show that the algorithm produces the correct output for $\sigma + 1$. Note that by assumption $ord\, \mathbf{P}_{l,\sigma} \geq \sigma$, i.e. its s-residual takes the form

$$\mathbf{P}_{l,\sigma}(z^s) \cdot \mathbf{F}(z) = z^\sigma \cdot R_l(z) \text{ with } R_l \in \mathbb{K}[[z]].$$

Hence $c_{l,\sigma} = R_l(0)$ and the recurrence step is well-defined. By construction we have

$$ord\, \mathbf{P}_{l,\sigma+1} \geq \sigma + 1 \text{ and } dct\, \mathbf{P}_{l,\sigma+1} \geq d_{l,\sigma+1} + 1.$$

Moreover, it is easy to see that with $\mathbf{P}_{1,\sigma}, \ldots, \mathbf{P}_{m,\sigma}$ also $\mathbf{P}_{1,\sigma+1}, \ldots, \mathbf{P}_{m,\sigma+1}$ are linearly independent with respect to polynomial coefficients.

Consider first the case when $\mathcal{L}_\delta^\sigma = \mathcal{L}_\delta^{\sigma+1}$. By assumption, each $\mathbf{Q} \in \mathcal{L}_\delta^{\sigma+1}$ then has a representation

$$\mathbf{Q} = \alpha_1 \cdot \mathbf{P}_{1,\sigma} + \ldots + \alpha_m \cdot \mathbf{P}_{m,\sigma}\ ,\ deg\ \alpha_l < dct\, \mathbf{P}_{l,\sigma} + \delta.$$

This is already a suitable linear combination of $\mathbf{P}_{1,\sigma+1}, \ldots, \mathbf{P}_{m,\sigma+1}$. To see this, notice that with $\alpha_l \neq 0$ we get $dct\, \mathbf{P}_{l,\sigma} + \delta > 0$ and $\mathbf{P}_{l,\sigma} \in \mathcal{L}_\delta^\sigma = \mathcal{L}_\delta^{\sigma+1}$, hence $c_{l,\sigma} = 0$ and $\mathbf{P}_{l,\sigma+1} = \mathbf{P}_{l,\sigma}$.

The case $\mathcal{L}_\delta^\sigma \neq \mathcal{L}_\delta^{\sigma+1}$ is also easy to handle. Let

$$\mathcal{L}_\delta := \{\alpha_1 \cdot \mathbf{P}_{1,\sigma+1} + \ldots + \alpha_m \cdot \mathbf{P}_{m,\sigma+1} \ :\ deg\ \alpha_l < dct\, \mathbf{P}_{l,\sigma+1} + \delta\},$$

so that in view of Lemma 3.3 we have $\mathcal{L}_\delta \subset \mathcal{L}_\delta^{\sigma+1}$. On the other hand, the dimension of $\mathcal{L}_\delta$ can be estimated as follows:

$$\begin{aligned} \dim \mathcal{L}_\delta &= \max\{dct\, \mathbf{P}_{1,\sigma+1} + \delta, 0\} + \ldots + \max\{dct\, \mathbf{P}_{m,\sigma+1} + \delta, 0\} \\ &\geq \max\{d_{1,\sigma+1} + 1 + \delta, 0\} + \ldots + \max\{d_{m,\sigma+1} + 1 + \delta, 0\} \\ &\geq \max\{d_{1,\sigma} + 1 + \delta, 0\} + \ldots + \max\{d_{m,\sigma} + 1 + \delta, 0\} - 1 \\ &= \dim \mathcal{L}_\delta^\sigma - 1 = \dim \mathcal{L}_\delta^{\sigma+1}, \end{aligned}$$

where for the last two equalities we have applied (7) and (10). Consequently, $\mathcal{L}_\delta = \mathcal{L}_\delta^{\sigma+1}$ and we have equality in the estimation above. For all $\Delta \geq \delta$ we also have that $\mathcal{L}_\Delta^{\sigma+1} \neq \mathcal{L}_\Delta^\sigma$, since by definition $\emptyset \neq \mathcal{L}_\delta^\sigma \setminus \mathcal{L}_\delta^{\sigma+1} \subset \mathcal{L}_\Delta^\sigma \setminus \mathcal{L}_\Delta^{\sigma+1}$. Therefore, the above equations are also valid if we replace δ by $\Delta \geq \delta$. Choosing Δ sufficiently large, we can conclude that $dct\, \mathbf{P}_{l,\sigma+1} = d_{l,\sigma+1} + 1$ for $l = 1, \ldots, m$ which proves the theorem. □

4 Some Properties of FPHPS Algorithm

In this section, we discuss some properties of the σ-bases obtained by the procedure FPHPS. In particular, we are interested in simple conditions describing whether some PHPA's are irreducible and whether given PHPA's $\mathbf{P}_1, \ldots, \mathbf{P}_\lambda$ (and its values at zero) are linearly independent with respect to polynomial coefficients (and constant coefficients, respectively) — questions which as explained in Section 2 naturally arise in the context of Matrix Padé approximation. In addition, for multidimensional solution sets we will classify PHPA's having 'best' approximation properties, i.e., maximal order and/or minimal degree. The complexity of method FPHPS is determined at the end of this section.

Let Λ_σ and π_σ (for a given σ) be defined as in Algorithm FPHPS. As given in all applications of Table 1, in the sequel we will only discuss the case $s \leq m$ and $\Lambda_0 \neq \{\}, \ldots, \Lambda_{s-1} \neq \{\}$. This is equivalent to the fact that the matrix $(\mathbf{F}(0), \mathbf{F}'(0), \ldots, \mathbf{F}^{(s-1)}(0))$ has full rank. In the following Theorem, we summarize some facts about reducible PHPA's. These results are generalizations of ideas appearing in [25].

Theorem 4.1.
(a) *For all $\sigma \geq s$, we have $card \Lambda_\sigma \geq 1$, more precisely*

$$\pi_{\sigma-s} \in \Lambda_\sigma \subset L_\sigma \cup \{\pi_{\sigma-s}\}, \text{ where } L_\sigma := \{1, \ldots, m\} \setminus \{\pi_{\sigma-s}, \pi_{\sigma-s+1}, \ldots, \pi_{\sigma-1}\}. \tag{11}$$

(b) *Let U denote the $(m-s)$ dimensional subspace of vectors which are orthogonal to all $\mathbf{F}(0), \mathbf{F}'(0), \ldots, \mathbf{F}^{(s-1)}(0)$. Then for $\sigma \geq s$*

$$span\{\mathbf{P}_{l,\sigma}(0) : l \in L_\sigma\} = U \quad \text{and for all } l \notin L_\sigma\text{:} \quad \mathbf{P}_{l,\sigma}(0) = 0. \tag{12}$$

Proof: Notice that in Algorithm FPHPS we always have $ord\, \mathbf{P}_{\pi_\sigma, \sigma+1} = \sigma + s$. Therefore $\pi_\sigma \in \Lambda_{\sigma+s} \neq \{\}$ but $\pi_\sigma \notin \Lambda_{\sigma+1}, \ldots, \pi_\sigma \notin \Lambda_{\sigma+s-1}$. This proves (a). The second part of (b) follows directly from the fact that $\mathbf{P}_{l,\sigma+1} = \mathbf{P}_{l,\sigma}$ for all $l \notin L_{\sigma+1} \cup L_\sigma$, and $\mathbf{P}_{l,\sigma+1}(0) = 0$ for $l = \pi_\sigma$. The first assertion of (b) can be shown by a simple recurrence argument on $\sigma \geq s$. Let

$$U_\sigma := span\{\mathbf{P}_{l,\sigma}(0) : l \in L_\sigma\}.$$

Then $U_\sigma \subset U$ since we have $ord\, \mathbf{P}_{l,\sigma} \geq s$. With $\mathbf{P}_{l,\sigma}(0)$, $l \in L_\sigma$, also the vectors $\mathbf{P}_{l,\sigma+1}(0)$, $l \in L_\sigma \cap L_{\sigma+1}$, together with $\mathbf{P}_{\pi_\sigma,\sigma}(0)$ are linearly independent. From the recurrence relations we know that $\mathbf{P}_{\pi_{\sigma-s},\sigma}(0) = 0$ and $\mathbf{P}_{\pi_{\sigma-s},\sigma+1}(0) = c \cdot \mathbf{P}_{\pi_\sigma,\sigma}(0)$ with $c \neq 0$. Consequently, $\mathbf{P}_{l,\sigma+1}(0)$, $l \in L_{\sigma+1}$, are linearly independent which proves part (b). □

Supposing that the vector $\mathbf{F}$ contains only polynomial entries, we expect that the solution set $\mathcal{L}_\delta^\sigma$ becomes stationary for sufficiently large σ. In contrast, due to Theorem 4.1(a) the σ-bases will always change if σ is increased. In fact, we observe that for large σ the non-constant part of the σ-basis described by the sets Λ_σ consists only of approximants with defect smaller than $-\delta$, and that, for sufficiently large σ, for the representation (6) of the solution set $\mathcal{L}_\delta^\sigma$ we need at most $(m-s)$ elements of the σ-basis.

Theorem 4.1(b) yields a simple criterion determining whether the solution set $\mathcal{L}_\delta^\sigma$ contains an irreducible element. By definition, the components of an element of the σ-basis can only have a common factor which vanishes at zero. Hence there exists an element $\mathbf{P}$ of $\mathcal{L}_\delta^\sigma$ being irreducible, i.e., $\mathbf{P}(0) \neq 0$, if and only if there is an $l \in L_\sigma$ with $d_{l,\sigma} \geq -\delta$. Moreover, we immediately get

Corollary 4.2.
(a) *$\mathcal{L}_\delta^\sigma$ contains $\lambda \leq m$ elements $\mathbf{P}_1, \ldots, \mathbf{P}_\lambda$ being linearly independent over $\mathbb{K}[z]$ iff there are distinct $l_1, \ldots, l_\lambda \in \{1, \ldots, m\}$ with $d_{l_j,\sigma} \geq -\delta$.*
(b) *$\mathcal{L}_\delta^\sigma$ contains $\lambda \leq m-s$ elements $\mathbf{P}_1, \ldots, \mathbf{P}_\lambda$ such that $\mathbf{P}_1(0), \ldots, \mathbf{P}_\lambda(0)$ are linearly independent over $\mathbb{K}$ iff there are distinct $l_1, \ldots, l_\lambda \in L_\sigma$ with $d_{l_j,\sigma} \geq -\delta$.*
(c) *In both cases linearly independent approximants from $\mathcal{L}_\delta^\sigma$ are given by $\mathbf{P}_j = \mathbf{P}_{l_j,\sigma}$, $j = 1, \ldots, \lambda$.* □

In most applications, the first s components of $\mathbf{F}$ take the simple form $f_j(z) = z^{j-1}$. Here we consider the first s components $\mathbf{p}$ and the last $(m-s)$ components $\mathbf{q}$ of a PHPA $\mathbf{P} = (\mathbf{p}, \mathbf{q})$ separately and ask for approximants $\mathbf{P}_1, \ldots, \mathbf{P}_\lambda \in \mathcal{L}_\delta^\sigma$ with $\mathbf{q}_1, \ldots, \mathbf{q}_\lambda$ (or $\mathbf{q}_1(0), \ldots, \mathbf{q}_\lambda(0)$) being linearly independent. Here also the criteria given in Corollary 4.2.(a),(b) can be applied as long as we can guarantee that there is no $\mathbf{P} = (\mathbf{p}, \mathbf{q}) \in \mathcal{L}_\delta^\sigma$ with $\mathbf{p} \neq 0$ and $\mathbf{q} = 0$ ($\mathbf{p}(0) \neq 0$ and $\mathbf{q}(0) = 0$, respectively). But due to the simple form of $\mathbf{F}$ it can be easily verified that $\mathbf{P} = (\mathbf{p}, \mathbf{q}) \in \mathcal{L}_\delta^\sigma$ with $\mathbf{q}(0) = 0$ and $\sigma \geq s$ also implies that $\mathbf{p}(0) = 0$. Similarly, if $s \cdot (n_j + \delta) + j \leq \sigma$ for $j = 1, \ldots, s$ (which for the most interesting PHPA cases of Section 2 is true) and $\mathbf{P} = (P_1, \ldots, P_m) = (\mathbf{p}, 0) \in \mathcal{L}_\delta^\sigma$ then $\mathbf{p}$ must also be identical zero since $ord\, \mathbf{P} \leq \max\{s \cdot deg\ P_j + j - 1 : j = 1, \ldots, s\}$.

If the solution set is multi-dimensional, we are interested in classifying particular solutions which have certain uniqueness properties. The concept of approximants with correct degree satisfying "best possible" order conditions is discussed in the following Corollary.

Corollary 4.3. *Let each* $\mathbf{P} \in \mathbb{K}^m[z]$ *have finite order and let* $\delta + \min\{n_1, \ldots, n_m\} \geq 0$. *Consider the problem of finding 'optimal' PHPA's* $\mathbf{P}_1, \ldots, \mathbf{P}_\lambda$, $\lambda \leq m - s$ *with*

(i) $\mathbf{P}_1(0), \ldots, \mathbf{P}_\lambda(0)$ *are linearly independent,*
(ii) $\text{dct } \mathbf{P}_1 > -\delta, \ldots, \text{dct } \mathbf{P}_\lambda > -\delta$,
(iii) the number $(\text{ord } \mathbf{P}_1 + \ldots + \text{ord } \mathbf{P}_\lambda)$ *is maximal,*
(iv) $\text{ord } \mathbf{P}_1 =: \sigma(1) > \text{ord } \mathbf{P}_2 =: \sigma(2) > \ldots > \text{ord } \mathbf{P}_\lambda =: \sigma(\lambda)$

(it is easy to see that condition (iv) only implies a particular ordering for the PHPA's determined by (i), (ii), (iii)). A solution for this problem is given by

$$\sigma(j) := \max\Big\{\sigma : card\{l \in L_\sigma : d_{l,\sigma} \geq -\delta\} \geq j\Big\}$$

and $\mathbf{P}_j = \mathbf{P}_{\pi_{\sigma(j)},\sigma(j)}$, $j = 1, \ldots, \lambda$. □

Corollary 4.3 is a canonical generalization of the optimal Hermite Padé form of type $\mathbf{n}(\delta)$ of [22] ($s = \lambda = 1$). Paszkowski speaks of non-existent optimal Hermite Padé forms if $\mathbf{P}_1$ is not unique, i.e., if there is a further (necessarily reducible) PHPA $\mathbf{P}_0$ with $dct\, \mathbf{P}_0 \geq -\delta$ and $ord\, \mathbf{P}_0 > ord\, \mathbf{P}_1$. For $\lambda = m - s = 1$, e.g., scalar simultaneous (partial) Padé approximation, our approach is closely connected to a concept proposed by de Bruin [8] for non-normal solution tables. Note that, though in view of Corollary 4.2.(b) the numbers $\sigma(1), \ldots, \sigma(\lambda)$ are unique, in general we might get several tuples of optimal PHPA's being essentially different. The significance of the integer $\sigma(\lambda)$ for Matrix Padé approximation is discussed at the end of Section 5.

Following Corollary 4.3, we always find irreducible approximants with correct degree, but the order condition might be weakened. In contrast, Van Barel and Bultheel [24, 26] look for irreducible approximants with correct order and a type of minimal degree. More precisely, instead of (ii)-(iv) the conditions

(v) $ord\, \mathbf{P}_1 \geq \sigma, \ldots, ord\, \mathbf{P}_\lambda \geq \sigma$,
(vi) the number $(dct\, \mathbf{P}_1 + \ldots + dct\, \mathbf{P}_\lambda)$ is maximal

are imposed. As above, in general this problem will not have a unique solution. However, the method FPHPS also gives a solution for this problem: due to Corollary 4.2(b) we can take those λ approximants $\mathbf{P}_{l,\sigma}$, $l \in L_\sigma$ with maximal defect.

The problem of uniqueness for both concepts is illustrated in the next example.

Example 4.4. Let

$$m = 4, \quad s = 2, \quad \mathbf{n} = (2, 2, 2, 2), \quad \delta = 0,$$
$$\mathbf{F}(z) = (1, z, \frac{z}{1 - z^4} + z^{10}, \frac{z}{1 + z^4} + z^{12})^T + \mathcal{O}(z^{16}).$$

An application of FPHPS gives the values $\pi_0, \pi_1, \ldots, \pi_{13} = 1,2,1,2,1,3,1,3,1,4,2,4,3,4$. In particular, we obtain a σ-basis for $\sigma = 10$ (output in matrix form with the rows $\mathbf{P}_{1,10}$, $\mathbf{P}_{2,10}$, $\mathbf{P}_{3,10}$, and $\mathbf{P}_{4,10}$ as the basis elements) as

$$\mathbf{P}_{10}(z) = \begin{bmatrix} z^5 & 0 & 0 & 0 \\ 0 & z^2 & -\frac{1}{2} & \frac{1}{2} \\ 0 & 1-z^2 & -\frac{1}{2}+z^2 & -\frac{1}{2} \\ 0 & -2z & z & z \end{bmatrix},$$

with s-residuals

$$\mathbf{P}_{10}(z^2)\cdot\mathbf{F}(z) = \begin{bmatrix} z^{10} + \mathcal{O}(z^{26}) \\ -\frac{z^{10}}{2} + \frac{z^{12}}{2} - z^{13} + \mathcal{O}(z^{16}) \\ -\frac{z^{10}}{2} - \frac{z^{12}}{2} + z^{13} + z^{14} + \mathcal{O}(z^{16}) \\ 2z^{11} + z^{12} + z^{14} + \mathcal{O}(z^{18}) \end{bmatrix}.$$

The defects for this basis are $-2,1,1$ and 2, respectively. Hence $\mathcal{L}_0^{10}$ does not have dimension 2 (as expected from comparing the number of equations and unknowns) but 4. For $\lambda = 1$, a particular solution with 'minimal degree' (satisfying conditions (i),(v),(vi) above) is given by $a \cdot \mathbf{P}_{2,10} + b \cdot \mathbf{P}_{3,10} + (cz + d)\cdot \mathbf{P}_{4,10}$ with arbitrary constants a, b, c, d, $|a| + |b| \neq 0$. A particular solution with 'maximal order' $\sigma(1) = 12$ (satisfying conditions (i),(ii),(iii),(iv) above) is given by $a \cdot \mathbf{P}_{3,12} + b \cdot \mathbf{P}_{4,12} = a\cdot(\mathbf{P}_{3,10} - \mathbf{P}_{2,10}) + b \cdot z \cdot \mathbf{P}_{4,10}$ with arbitrary constants a, b, $a \neq 0$ (the solution proposed in Corollary 4.3 equals $\mathbf{P}_{3,12}$). □

Consider now the problem of determining the complexity of the algorithm FPHPS. For simplicity, we still impose the conditions before Theorem 4.1 (otherwise, the complexity will be still smaller). As seen in Section 2, in most applications one has to determine σ-bases of PHPA's for $\sigma \approx \|\mathbf{n}\|$. In order to determine the number of arithmetic operations (AO) required for the computation of a $\|\mathbf{n}\|$-basis, we essentially only have to take into account the computation of $c_{1,\sigma}, \ldots, c_{m,\sigma}$ and of $\mathbf{P}_{1,\sigma+1}, \ldots, \mathbf{P}_{m,\sigma+1}$, $0 \leq \sigma < \|\mathbf{n}\|$. Here the complexity strongly depends on the parameters $\mathbf{F}$ and s.

Theorem 4.5. (Complexity) *The algorithm FPHPS for computing PHPA's of order $\sigma = 0, 1, \ldots, \|\mathbf{n}\|$ has a complexity of at most*

$$4(m-s)\cdot\|\mathbf{n}\|^2 + \mathcal{O}(m^2 \cdot \|\mathbf{n}\|)\ AO, \tag{13}$$

roughly half additions and half multiplications plus $\mathcal{O}(m \cdot \|\mathbf{n}\|)$ divisions. At least for the case $\mathbf{n} = (n, \ldots, n)$, we obtain the sharper bound

$$(1 - \frac{s}{m})\cdot(2m - \text{card}\ L)\cdot\|\mathbf{n}\|^2 + \mathcal{O}(m^2\cdot\|\mathbf{n}\|)\ AO, \tag{14}$$

where $L = \{l : f_l(z) = z^j$ with a $j \in \mathbb{N}_0\}$.

Proof: Since $c_{\pi_{\sigma-s},\sigma} = c_{\pi_{\sigma-s},\sigma-s}$ and $P_{\pi_\sigma,\sigma+1}$ can be easily determined by shifting some coefficients, for the complexity it remains to consider the computation of at most $c_{l,\sigma}$

and $\mathbf{P}_{l,\sigma+1}$ for $l \in L_{\sigma+1}$. In addition, we are not interested in PHPA's with $dct\, \mathbf{P}_{l,\sigma} \leq 0$, since they do not occur in the solution sets $\mathcal{L}_\delta^\sigma$, $\delta \leq 0$ (cf. Eqn (6)). Therefore the degree of the λth component of $\mathbf{P}_{l,\sigma}$ is bounded by $n_\lambda - d_{l,\sigma} \leq n_\lambda$ and we require for loop no. σ the number of at most $2 \cdot \sum_{l \in L_{\sigma+1}} \sum_{\lambda=1}^m (n_\lambda + 1) + \mathcal{O}(m^2) = 2(m-s) \cdot \|\mathbf{n}\| + \mathcal{O}(m^2)$ additions/subtractions and the same number of multiplications which totally gives a complexity as stated in (13). For the case $\mathbf{n} = (n, \ldots, n)$, we can apply the relation

$$2 \cdot \sum_{\sigma=0}^{\|\mathbf{n}\|-1} \sum_{l \in L_{\sigma+1}} (d_{l,\sigma} + 1) \geq \ldots \geq \|\mathbf{n}\|^2 - 2 \cdot s \cdot \sum_{l=1}^{m} \sum_{j=0}^{n+1} j.$$

which by using similar arguments leads to (14). □

It should be mentioned that our algorithm can be implemented very efficiently on a vector or on a parallel processor (with, e.g., m or $\|\mathbf{n}\|$ processors). The complexity of our algorithm for the examples of Section 2 is given in Table 2, whereas in Table 3 some solved subproblems and their corresponding PHPA solution space are listed.

Example	Complexity via (13)	via (14), special case
classical Hermite Padé	$4(m-1) \cdot \|\mathbf{n}\|^2 + \mathcal{O}(m^2 \cdot \|\mathbf{n}\|)$	for $n_1 = \ldots = n_m$: $2(m-1) \cdot \|\mathbf{n}\|^2 + \mathcal{O}(m^2 \cdot \|\mathbf{n}\|)$
2.1	$4q[p(M+1) + q(N+1)]^2 + \mathcal{O}((p+q)^2 \cdot (M+N))$	for $M = N$: $q(2q+p)(p+q)(M+1)^2 + \mathcal{O}((p+q)^2 \cdot M)$
2.2	$4p[q(M+1) + p(N+1)]^2 + \mathcal{O}((p+q)^2 \cdot (M+N))$	for $M = N$: $p(2p+q)(p+q)(M+1)^2 + \mathcal{O}((p+q)^2 \cdot M)$
2.3	$4\mu p^3 \rho^2 + \mathcal{O}(\mu^2 p^4 \rho)$	for $\rho_0 = \ldots = \rho_\mu$: $2\mu p^3 \rho^2 + \mathcal{O}(\mu^2 p^4 \rho)$
2.4 with $p = 1, A_0 = 1$	$4\mu^2 \rho^2 + \mathcal{O}(\mu^4 \rho)$	for $\rho_0 = \ldots = \rho_\mu$: $\frac{\mu+2}{\mu+1} \mu^2 \rho^2 + \mathcal{O}(\mu^4 \rho)$

TABLE 2: Complexity for solving Matrix-type Padé Approximation problems

Example	Type of subproblem	PHPA solution space
classical Hermite Padé	$(n_1-j,\ldots,n_m-j)$, $j\le\min\{n_l+1\}$	$\mathcal{L}_{-j}^{\sigma-j\cdot m}$
2.1	$(M-j,N-j)$, $j\le\min\{M+1,N+1\}$	$\mathcal{L}_{-j}^{\sigma-2\cdot j\cdot s}$ contains rows of (P^T,Q^T)
2.2	$(M-j,N-j)$, $j\le\min\{M+1,N+1\}$	$\mathcal{L}_{-j}^{\sigma-2\cdot j\cdot s}$ contains rows of (P,Q)
2.3	$(\rho_0-j,\ldots,\rho_\mu-j)$, $j\le\min\{\rho_l\}$	$\mathcal{L}_{-j}^{\sigma-j\cdot m}$ contains rows of $(P_0,\ldots,P_\mu)$
2.4 with $p=1, A_0=1$	$(\rho_0-j,\ldots,\rho_\mu-j)$, $j\le\min\{\rho_l\}$	$\mathcal{L}_{-j\cdot s}^{\sigma-j\cdot s\cdot m}$

TABLE 3: Some Matrix-type Padé subproblems solved by FPHPS and their corresponding PHPA solution spaces, parameters $m,\mathbf{n},s,\sigma,\mathbf{F}$ as in Table 1

5 An Example of Matrix Padé Approximation

In this section we give an example of a matrix Padé approximation problem computed using the algorithm FPHPS. Let

$$A(z)=\begin{bmatrix} 1+z^2+2z^4-z^5+z^6+\mathcal{O}(z^8) & z^7+\mathcal{O}(z^8) \\ -z^5+\mathcal{O}(z^8) & 1+z^2+z^4+z^7+\mathcal{O}(z^8)\end{bmatrix}$$

and consider the problem of determining a (2,3) right-hand matrix Padé form for $A(z)$. Thus we are looking for 2×2 matrix polynomials P and Q of degree at most 2 and 3, respectively, such that

$$A(z)\cdot Q(z)-P(z)=z^6\cdot R(z)$$

for some matrix power series R. The suitable choice of the parameters is stated in Table 1, row 2. Notice that, for any PHPA (P_1,P_2,P_3,P_4) of type $((M,M,N,N),2(M+N+1),2)$, the components P_1 and P_2 correspond to a column of an (M,N) right-hand matrix Padé numerator while P_3, P_4 correspond to a column of the denominator (cf. Table 3, for left-hand matrix Padé approximation, P_1, P_2 and P_3, P_4 correspond to rows of numerator and denominator, respectively).

Setting $s=2$, $\mathbf{n}=(2,2,3,3)$ and

$$\begin{aligned}\mathbf{F}^T(z) &= [1,z]\cdot\left[\mathbf{I},-A(z^2)\right]\\ &= \left[1,z,-1-z^4-2z^8+z^{10}+z^{11}-z^{12}+\mathcal{O}(z^{16}),-z-z^5-z^9-z^{14}-z^{15}+\mathcal{O}(z^{16})\right]\end{aligned}$$

and using the algorithm FPHPS gives a σ-basis for $\sigma=12$ (output in matrix form with the rows as the basis elements) as

$$\begin{bmatrix} -z-z^2+z^3 & 0 & -z-z^2+2z^3+z^4 & 0 \\ 1+z-z^2 & z^3 & 1+z-2z^2-z^3 & z^3 \\ -z^2 & 0 & -z^2+z^4 & 0 \\ 0 & -1 & 0 & -1+z^2 \end{bmatrix}.$$

The defects for this basis are $0,0,0$ and 2, respectively. Therefore a basis for the solution space $\mathcal{L}_0^{12}$, as a finite-dimensional space over $\mathbb{K}$, is given by $(a+b\cdot z)\cdot \mathbf{P}_{4,12}=(a+b\cdot z)\cdot [0,-1,0,-1+z^2]$ with a and b being arbitrary constants. Translating the solution space basis into matrix form implies that the columns of P and Q are generated by

$$(a+bz)\cdot \begin{bmatrix} 0 \\ -1 \end{bmatrix} \quad \text{and} \quad (a+bz)\cdot \begin{bmatrix} 0 \\ -1+z^2 \end{bmatrix},$$

respectively. This gives a right matrix Padé form of type $(2,3)$ for $A(z)$ as

$$P(z)=\begin{bmatrix} 0 & 0 \\ -1 & -z \end{bmatrix} \quad \text{and} \quad Q(z)=\begin{bmatrix} 0 & 0 \\ -1+z^2 & -z+z^3 \end{bmatrix}.$$

In this case, such a matrix Padé form is unique up to multiplication on the right by a non-singular 2×2 matrix. In particular, notice that it is not possible to construct a right matrix Padé fraction of type $(2,3)$ in this instance.

The left matrix Padé forms of type $(2,3)$ for $A(z)$ can also be computed by the FPHPS procedure. Setting $s=2$, $\mathbf{n}=(2,2,3,3)$ and

$$\mathbf{F}(z)=\begin{bmatrix} \mathbf{I} \\ -A(z^2) \end{bmatrix}\cdot\begin{bmatrix} 1 \\ z \end{bmatrix}=\begin{bmatrix} 1 \\ z \\ -1-z^4-2z^8+z^{10}+\mathcal{O}(z^{12}) \\ -z-z^5-z^9+z^{10}+\mathcal{O}(z^{12}) \end{bmatrix},$$

and computing the σ-basis for $\sigma=12$ gives

$$\begin{bmatrix} -1+z^2 & 1 & -1+2z^2 & 1-z^2 \\ 0 & z^4 & 0 & z^4 \\ -z & -1 & -z+z^3 & -1+z^2 \\ 0 & -z & 0 & -z+z^3 \end{bmatrix}.$$

In this case the defects are $1,-1,1$ and 1, respectively, so the solution space $\mathcal{L}_0^{12}$ is of the form $a\cdot\mathbf{P}_{1,12}+b\cdot\mathbf{P}_{3,12}+c\cdot\mathbf{P}_{4,12}$ with a,b and c arbitrary constants. Again translating the basis information to matrix form implies that the rows of P and Q are generated by

$$a\cdot[-1+z^2,1]+b\cdot[-z,-1]+c\cdot[0,-z]$$

and

$$a\cdot[-1+2z^2,1-z^2]+b\cdot[-z+z^3,-1+z^2]+c\cdot[0,-z+z^3]$$

respectively. Unlike the previous example, there is not one Padé form that is unique up to left multiplication by a nonsingular matrix of scalars. One possibility for a left matrix Padé form in this case is

$$P(z) = \begin{bmatrix} -z & -1 \\ -1+z^2 & 1 \end{bmatrix} \quad \text{and} \quad Q(z) = \begin{bmatrix} -z+z^3 & -1+z^2 \\ -1+2\,z^2 & 1-z^2 \end{bmatrix}.$$

Notice that the denominator has a non-zero determinant, indeed that $Q(0)$ is non-singular. Therefore, unlike the case for approximants on the right, one can always form the rational expression $Q(z)^{-1} \cdot P(z)$.

Using the algorithm FPHPS in the above example also determines, at no added cost, the σ-basis for $\mathcal{L}^{4}_{-2}$ and $\mathcal{L}^{8}_{-1}$. Hence the right matrix Padé forms of type $(0,1)$

$$P(z) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad Q(z) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and $(1,2)$

$$P(z) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, \quad Q(z) = \begin{bmatrix} -1+z^2 & 0 \\ 0 & -1+z^2 \end{bmatrix}$$

(determined uniquely up to matrix multiplication on the right in both cases) are by-products of the previous computation. In addition, one can continue the computation to determine the matrix Padé form of type $(3,4)$ since the σ-basis for $\mathcal{L}^{12}_{0}$ can be used to determine the σ-basis for $\mathcal{L}^{16}_{1}$. In the case of the right matrix Padé form of type $(3,4)$ this gives (again unique up to matrix multiplication on the right)

$$P(z) = \begin{bmatrix} 0 & 1+z/5+11/5z^2+4/5z^3 \\ -z^2 & 1/5-2/5z+z^3 \end{bmatrix},$$

$$Q(z) = \begin{bmatrix} 0 & 1+z/5+6/5z^2+3/5z^3-16/5z^4 \\ -z^2+z^4 & -1/5-2/5z+1/5z^2+7/5z^3 \end{bmatrix},$$

an example where the denominator matrix polynomial Q is nonsingular but has a singular leading term $Q(0)$.

Our example shows that, in general, the matrix Padé approximation problem does not have a unique rational solution like in the scalar case. Moreover, there are three distinct and possible forms of a denominator matrix polynomial Q. First, the case occurs when $Q(z)$ is singular for all z and hence no matrix rational form exists, this type of degeneracy is not found in the scalar case. Secondly, it is possible that $Q(0)$ is non-singular (cf. Corollary 4.2(a),(b) and the following remarks). Here we can form $P(z) \cdot Q(z)^{-1}$ and its matrix power series agrees with $A(z)$ to the full order condition. Finally, if $Q(z)$ is non-singular for some z but $Q(0)$ is singular, we can cancel P and Q by a common matrix polynomial factor on the right. Here, similarly to the degenerate case found in scalar Padé approximation, the resulting matrix rational form $P(z) \cdot Q(z)^{-1}$ does not agree anymore with $A(z)$ to the full order condition.

Note that the concept as proposed in Corollary 4.3 ($2\lambda = 2s = m$) always leads to a matrix Padé-like form with correct degree and maximal order $[\frac{\sigma(s)}{s}]$ (perhaps less than $(M+N+1)$ as required for matrix Padé approximants) where by forming the rational function $P(z) \cdot Q(z)^{-1}$ we do not obtain an additional order deflation. In fact one can show that there is no other rational function of the form $P(z) \cdot Q(z)^{-1}$ satisfying the degree constraints and having an order greater than $[\frac{\sigma(s)}{s}]$.

6 A superfast PHPA solver

In Section 4 we have shown that algorithm FPHPS computes a σ-basis with quadratic complexity. This is better than using methods such as Gaussian elimination and is optimal in special cases for arbitrary fields $\mathbb{K}$. However, when the field $\mathbb{K}$ allows for fast polynomial multiplication via the use of the FFT (cf. [15]) then there are faster methods in special cases. For example, when $s = 1$ and $m = 2$ (i.e. the case of Padé approximation) the algorithms of Brent, Gustavson and Yun [9] and Cabay and Choi [10] compute these approximants with the superfast complexity $\mathcal{O}(\sigma \log^2 \sigma)$. Similarly, a recent algorithm of Cabay and Labahn [12] also solves the Hermite Padé and simultaneous Padé problems with superfast complexity. In this section we describe a second algorithm that takes advantage of fast polynomial multiplication when solving the PHPA problem. The new algorithm has the advantage of always being superfast - the algorithm of [12] sometimes slows down to quadratic or even cubic complexity (if most of the subproblems of type $\mathbf{n}(\delta)$, $\delta < 0$ do not have a unique solution) although in practical problems this is rare.

Algorithm FPHPS of Section 3 provides a σ-basis $\mathbf{P}_1, \ldots, \mathbf{P}_m$ with respect to given $\mathbf{F}$, $\mathbf{n}$ and σ (and a fixed parameter s). For convenience, we arrange the $\mathbf{P}_l = (P_{l,1}, \ldots, P_{l,m})$ in a matrix $\mathbf{P} = (P_{l,\lambda})_{l=1,\ldots,m}^{\lambda=1,\ldots,m}$. Then with $\mathbf{d} := (d_1, \ldots, d_m)$, $d_l := dct\, \mathbf{P}_l - 1$, we can symbolize the procedure as follows

$$(\mathbf{P}, \mathbf{d}) \longleftarrow \text{ FPHPS } (\mathbf{F}, \sigma, \mathbf{n}).$$

Note that, in general, the choice of π_σ and therefore the output of FPHPS is not unique, but uniqueness could be easily obtained for instance by the additional restriction that π_σ has to be as small as possible.

The basic step of a divide-and-conquer version is described in the next Theorem.

Theorem 6.1. *Let ρ, σ be integers with $0 \le \rho \le \sigma$. Suppose that we have iterated $\rho \le \sigma$ times the recursive step of FPHPS*

$$(\mathbf{P}^{(1)}, \mathbf{d}^{(1)}) \longleftarrow \textit{ FPHPS}(\mathbf{F}, \rho, \mathbf{n}),$$

and then continue iterating

$$(\mathbf{P}^{(3)}, \mathbf{d}^{(3)}) \longleftarrow \textit{FPHPS}(\mathbf{F}, \sigma, \mathbf{n}).$$

Suppose further that we restart the procedure with new initializations

$$(\mathbf{P}^{(2)}, \mathbf{d}^{(2)}) \longleftarrow \textit{FPHPS}(\mathbf{F}^{(1)}, \sigma - \rho, \mathbf{d}^{(1)}), \text{ where } \mathbf{F}^{(1)}(z) := z^{-\rho} \cdot \mathbf{P}^{(1)}(z^s) \cdot \mathbf{F}(z),$$

where we always use the above uniqueness condition for the values π_σ. Then

$$\mathbf{P}^{(3)} = \mathbf{P}^{(2)} \cdot \mathbf{P}^{(1)} \quad \textit{and} \quad \mathbf{d}^{(3)} = \mathbf{d}^{(2)}.$$

Proof: We show Theorem 6.1 by induction on $(\sigma - \rho)$. Extending our notation slightly, set

$$(\mathbf{P}^{(1)}_\rho, \mathbf{d}^{(1)}_\rho) = (\mathbf{P}^{(1)}, \mathbf{d}^{(1)}), \quad (\mathbf{P}^{(3)}_\sigma, \mathbf{d}^{(3)}_\sigma) = (\mathbf{P}^{(3)}, \mathbf{d}^{(3)}), \quad (\mathbf{P}^{(2)}_{\sigma-\rho}, \mathbf{d}^{(2)}_{\sigma-\rho}) = (\mathbf{P}^{(2)}, \mathbf{d}^{(2)}).$$

Note that the Theorem is trivially true for $\sigma - \rho = 0$. Assume now that the result is true for $\sigma - \rho \geq 0$. Then

$$\mathbf{P}^{(3)}_\sigma = \mathbf{P}^{(2)}_{\sigma-\rho} \cdot \mathbf{P}^{(1)}_\rho \quad \text{and} \quad \mathbf{d}^{(3)}_\sigma = \mathbf{d}^{(2)}_{\sigma-\rho}. \tag{15}$$

Consequently, the corresponding s-residuals

$$\mathbf{R}^{(3)}_\sigma(z) = z^{-\sigma} \cdot \mathbf{P}^{(3)}_\sigma(z^s) \cdot \mathbf{F}(z) \quad \text{and} \quad \mathbf{R}^{(2)}_{\sigma-\rho}(z) = z^{-\sigma+\rho} \cdot \mathbf{P}^{(2)}_{\sigma-\rho}(z^s) \cdot \mathbf{F}^{(1)}(z)$$

are equal. Hence in both cases we have to take the same value π and the assertion (15) with σ replaced by $(\sigma + 1)$ follows. □

The basic step of a divide-and-conquer version (15) yields the *Superfast Power Hermite Padé Solver* SPHPS, a reliable algorithm for computing a σ-basis of PHPA's with complexity $\mathcal{O}(\sigma \cdot \log^2 \sigma)$. The reason for the improvement in complexity results from the use of Fast-Fourier-Transform (FFT) techniques for fast polynomial multiplication. Such techniques consist of converting to a new coordinate representation via polynomial evaluation at roots of unity, computing the arithmetic operations in these new coordinates and transfering the results back to the original computation domain via polynomial interpolation. For purposes of efficiency we describe our superfast algorithm in both coordinate representations. Hence we will require some FFT details needed for our implementation. Additional details of the FFT procedure can be found in many texts (cf., [15]).

Let ω_κ be the principal κth root of unity (for example, if $\mathbb{K}$ is the complex numbers then $\omega_\kappa := \cos(\frac{2\pi}{\kappa}) + i \cdot \sin(\frac{2\pi}{\kappa})$) and let

$$(\xi_j)_{j=0,\ldots,2\kappa-1} \longleftarrow DFT_{2\kappa}(p(z))$$

denote the evaluation of $\xi_j := p(\omega^j_{2\kappa})$, $j = 0, \ldots, 2\kappa - 1$. Then for the classical discrete FFT-algorithm we split p into its even and odd part $p(z) = p_e(z^2) + z \cdot p_o(z^2)$ and use the fact that for $j = 0, \ldots, \kappa - 1$ we have

$$\xi_j = \xi^{(e)}_j + \omega^j_{2\kappa} \cdot \xi^{(o)}_j \text{ and } \xi_{\kappa+j} = \xi^{(e)}_j - \omega^j_{2\kappa} \cdot \xi^{(o)}_j$$

where $(\xi_j^{(e)})_{j=0,\ldots,\kappa-1} \longleftarrow DFT_\kappa(p_e(z))$ and $(\xi_j^{(o)})_{j=0,\ldots,\kappa-1} \longleftarrow DFT_\kappa(p_o(z))$. The 'inverse' polynomial interpolation computation of

$$p(z) \longleftarrow IDFT_\kappa((\xi_j)_{j=0,\ldots,\kappa-1}),$$

i.e. of the uniquely defined polynomial p of degree less than κ with $\xi_j := p(\omega_\kappa^j)$, $j = 0, \ldots, \kappa - 1$, is done by

$$\hat{p}(z) := \sum_{j=0}^{\kappa-1} \xi_j z^{n-j}, (\hat{\xi}_j)_{j=0,\ldots,\kappa-1} \longleftarrow DFT_\kappa(\hat{p}(z)), \text{ then } p(z) = \frac{1}{\kappa} \cdot \sum_{j=0}^{\kappa-1} \hat{\xi}_j z^j.$$

Polynomials are multiplied componentwise in the new coordinates, that is, if

$$\begin{aligned}
&(\xi_j^{(1)})_{j=0,\ldots,\kappa-1} \longleftarrow DFT_\kappa(p_1(z)), \\
&(\xi_j^{(2)})_{j=0,\ldots,\kappa-1} \longleftarrow DFT_\kappa(p_2(z)), \quad \text{and} \\
&p^{(3)}(z) \longleftarrow IDFT_\kappa((\xi_j^{(1)} \cdot \xi_j^{(2)})_{j=0,\ldots,\kappa-1}),
\end{aligned}$$

and if c denotes the leading coefficient of $p_1(z) \cdot p_2(z)$, then

$$\begin{aligned}
p^{(3)}(z) &= p^{(1)}(z) \cdot p^{(2)}(z) \bmod z^\kappa \\
&= p^{(1)}(z) \cdot p^{(2)}(z) + \begin{cases} 0 & \text{if } deg\ (p^{(1)} \cdot p^{(2)}) < \kappa, \\ -c \cdot z^\kappa + c & \text{if } deg\ (p^{(1)} \cdot p^{(2)}) = \kappa. \end{cases}
\end{aligned}$$

For κ a power of two, the complexity of converting to the new coordinate representation and back again (via either DFT_κ or $IDFT_\kappa$) is at most $\frac{1}{2} \cdot \kappa \cdot \log \kappa + \mathcal{O}(\kappa)$ multiplications and $\kappa \cdot \log \kappa + \mathcal{O}(\kappa)$ additions (the logarithm taken with respect to the basis 2). Therefore the polynomial multiplication is of complexity $\mathcal{O}(\kappa \cdot \log \kappa)$.

In the SPHPS algorithm, we use the notations: $\mathbf{e}_l$ is the lth unit vector, $\mathbf{I}$ the unit matrix of size $(m \times m)$ and $\left\{\sum_{j=0}^{\infty} c_j z^j\right\}_\kappa := \sum_{j=0}^{\kappa-1} c_j z^j$ denotes a truncated power series.

ALGORITHM SPHPS $(\mathbf{F}, \sigma, \kappa, \mathbf{n})$

INPUT: $\sigma, \kappa \in \mathbb{N}_0$, with $\sigma \leq \kappa = 2^k$ for a $k \in \mathbb{N}_0$,

$\mathbf{n} = (n_1, \ldots, n_m)$, vector of integers,

$\mathbf{F} = (f_1, \ldots, f_m)^T$ vector of truncated power series,

i.e. of polynomials of degree less than κ,

Let $\mathbf{G} \in \mathbb{K}^{m \times s}[z]$ be defined by $\mathbf{F}(z) = \mathbf{G}(z^s) \cdot (1, z, \ldots, z^{s-1})^T$

OUTPUT: $\mathbf{P}$, ξ and $\mathbf{d}$ where:

$\mathbf{d} = (d_1, \ldots, d_m)$, vector of integers,

$\mathbf{P} = (P_{l,\lambda})_{l=1,\ldots,m}^{\lambda=1,\ldots,m}$, consisting of rows

$\mathbf{P}_l = (P_{l,1}, \ldots, P_{l,m})$ with $dct\ \mathbf{P}_l = d_l + 1$,

$deg\ P_{l,l} \leq \kappa$ and for $l \neq \lambda$: $deg\ P_{l,\lambda} < \kappa$,

for all $\delta \in \mathbb{Z}$: $\mathcal{L}_\delta^\sigma = \{\alpha_1 \mathbf{P}_1 + \ldots + \alpha_m \mathbf{P}_m : deg\ \alpha_l \leq d_l + \delta\}$

$\xi = (\xi_j)_{j=0,\ldots,2\kappa-1}$, each ξ_j an m by m matrix,

$(\xi_j)_{j=0,\ldots,2\kappa-1} \longleftarrow DFT_{2\kappa}(\mathbf{P}(z))$

THE RECURSION:

CASE ($\sigma = 0$ and $\kappa \geq 1$) OR ($\sigma = \kappa = 1$ and $f_1(0) = \ldots = f_m(0) = 0$):

RETURN $(\mathbf{P}, \xi, \mathbf{d}) = (\mathbf{I}, \underbrace{(\mathbf{I}, \ldots, \mathbf{I})}_{2\kappa}, \mathbf{n})$

CASE $\sigma = \kappa = 1$, $f_\pi(0) \neq 0$ and for all l with $n_l > n_\pi$: $f_l(0) = 0$:

$$\mathbf{P} \longleftarrow \begin{bmatrix} 1 & & & -f_1(0)/f_\pi(0) & & & \\ & \ddots & & \vdots & & & \\ & & 1 & -f_{\pi-1}(0)/f_\pi(0) & & & \\ & & & z & & & \\ & & & -f_{\pi+1}(0)/f_\pi(0) & 1 & & \\ & & & \vdots & & \ddots & \\ & & & -f_m(0)/f_\pi(0) & & & 1 \end{bmatrix}$$

RETURN $(\mathbf{P}, \xi, \mathbf{d}) = (\mathbf{P}, (\mathbf{P}(1), \mathbf{P}(-1)), \mathbf{n} - \mathbf{e}_\pi)$

CASE $\sigma \geq 1$ and $\kappa > 1$: (Divide-and-Conquer step)

Compute basis to order $\kappa/2$:

$\overline{\kappa} \longleftarrow \kappa/2$, $\overline{\sigma} \longleftarrow \min\{\sigma, \overline{\kappa}\}$; $\mathbf{F}^{(1)}(z) \longleftarrow \{\mathbf{F}(z)\}_{\overline{\kappa}}$

$(\mathbf{P}^{(1)}, \xi^{(1)}, \mathbf{d}^{(1)}) \longleftarrow$ SPHPS $(\mathbf{F}^{(1)}, \overline{\sigma}, \overline{\kappa}, \mathbf{n})$

Compute basis to order κ:

$(\eta_j)_{j=0,\ldots,\kappa-1} \longleftarrow DFT_\kappa(\mathbf{G}(z))$

$\mathbf{G}^{(2)}(z) \longleftarrow IDFT_\kappa((\xi_j^{(1)} \cdot \eta_j)_{j=0,\ldots,\kappa-1})$

$\mathbf{F}^{(2)}(z) \longleftarrow \{z^{-\overline{\kappa}} \cdot \mathbf{G}^{(2)}(z^s) \cdot (1, z, \ldots, z^{s-1})^T\}_{\overline{\kappa}}$

$(\mathbf{P}^{(2)}, \xi^{(2)}, \mathbf{d}^{(2)}) \longleftarrow$ SPHPS $(\mathbf{F}^{(2)}, \sigma - \overline{\sigma}, \overline{\kappa}, \mathbf{d}^{(1)})$

Combine both parts:

$\xi_{2j}^{(3)} \longleftarrow \xi_j^{(2)} \cdot \xi_j^{(1)}$ for $j = 0, 1, \ldots, \kappa - 1$

$\mathbf{P}^{(3)}(z) \longleftarrow IDFT_\kappa((\xi_{2j}^{(3)})_{j=0,\ldots,\kappa-1})$

If $deg\ P_{l,l}^{(1)} = deg\ P_{l,l}^{(2)} = \overline{\kappa}$, then $P_{l,l}^{(3)}(z) \longleftarrow P_{l,l}^{(3)}(z) - 1 + z^\kappa$

$(\xi_{2j+1}^{(3)})_{j=0,1,\ldots,\kappa-1} \longleftarrow DFT_\kappa(\mathbf{P}^{(3)}(\omega_{2\kappa} \cdot z))$

RETURN $(\mathbf{P}, \xi, \mathbf{d}) = (\mathbf{P}^{(3)}, \xi^{(3)}, \mathbf{d}^{(2)})$

Consider now the problem of determining the complexity of the SPHPS algorithm. For simplicity, we still impose the conditions before Theorem 4.1 (otherwise, the complexity will be still smaller). As seen in Section 2, in most applications one has to determine σ-bases of PHPA's for $\sigma \approx \|\mathbf{n}\|$.

Theorem 6.2. (Complexity) *The algorithm SPHPS for computing PHPA's of order σ has a complexity of at most*

$$\frac{3}{2} \cdot (m+s) \cdot m \cdot \sigma \cdot \log^2 \sigma + \mathcal{O}(\sigma \cdot \log \sigma) \; AO, \tag{16}$$

roughly half multipications as additions.

Proof: Let $\Phi_A(\kappa)$ and $\Phi_M(\kappa)$ denote the number of additions/subtractions and multiplications/divisions required for algorithm SPHPS with parameter κ, respectively. We easily obtain $\Phi_A(1) \leq 1$ and $\Phi_M(1) \leq m-1$. Moreover, in the last case we call the subroutines DFT_κ or $IDFT_\kappa$ at most $2(m+s)m$ times, hence

$$\Phi_A(\kappa) \leq 2 \cdot \Phi_A(\kappa/2) + 2 \cdot (m+s) \cdot m \cdot \kappa \cdot \log \kappa + \mathcal{O}(\kappa)$$

and

$$\Phi_M(\kappa) \leq 2 \cdot \Phi_M(\kappa/2) + (m+s) \cdot m \cdot \kappa \cdot \log \kappa + \mathcal{O}(\kappa).$$

This gives the complexity result. □

We remark that, as was the case with method FPHPS, the complexity will be even less for some special cases. For example, for simultaneous Padé approximation, this number will be smaller if one carefully checks whether some entries of the matrix $\mathbf{G}$ always equal zero or 1.

7 Conclusions

In this paper we have studied the concept of a Power Hermite Padé Approximant. These approximants are shown to generalize a number of Padé approximation problems including for example the classical Hermite Padé and simultaneous Padé approximation problems as well as matrix-type generalizations of common Padé approximation problems. A fast (and also a superfast), reliable algorithm to compute these approximants is given. In this way our work provides a uniform method of both describing and computing a wide variety of Padé and matrix-Padé approximation problems. As an immediate application, our work results in new and faster algorithms for a number of problems that rely on matrix-type Padé computation. For example our algorithms, used in conjunction with the results of [17] gives faster algorithms for the inversion of striped or layered block Hankel (or Toeplitz) matrices. Similarly the same algorithms combined with the results of [18] give similar improvements for the inversion of rectangular-block Hankel (or Toeplitz) matrices.

There are a number of directions for new research in this area. Our algorithm follows an m-dimensional "diagonal" path. In special cases, however, fast, reliable algorithms are given (cf., [4]) that can succeed on arbitrary staircase paths in m-dimensional space. The methods of [4] could also be extended to compute the more general PHPA's on arbitrary staircase paths, leading to a method with smaller complexity (cf., [26]).

Our algorithm does not consider the problem of stability when the computations are to be done with floating point numbers. Recently Cabay and Meleshko [13] have presented a (weakly) stable algorithm for the case $s = 1$ and $m = 2$. We conjecture that such an algorithm is also possible for the PHPA problem with arbitrary s and m, though not necessarily using the same approach as used in this paper. Our algorithm assumes exact arithmetic and has been implemented in the Maple computer algebra system. However it does not consider the problem of exponential growth of the coefficients resulting in our computations. It would be of interest to extend our algorithm to this case. This would be done by restricting $\mathbb{K}$ to be an integral domain rather than a field and perhaps using fraction-free methods similar to that used for solving polynomial gcd problems (cf., [15]).

Finally, the concept of a PHPA is a scalar generalization of a Hermite-Padé approximant used to solve matrix-like Padé approximation problems. As shown in [5] this concept also allows, for example, for a description of the structures in a singular PHPA solution table by adapting the scalar techniques of [3]. For matrix-like rational interpolation problems (with arbitrary knots), a common framework is given by the vector M-Padé approximation as a canonical extension of Example 2.5 (see [26]). In contrast, we are interested in a scalar generalization of the M-Padé approximant which can be used for simple, fast and efficient algorithms, and which — following [3, 5] — might also be helpful for obtaining results about the structure of the singular matrix rational interpolation table.

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