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The Need for Knowledge and Reliability in Numeric Computation: Case Study of Multivariate Padé Approximation

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Abstract. In this paper we review and link the numeric research projects carried out at the Department of Mathematics and Computer Science of the University of Antwerp since 1978. Results have and are being obtained in various areas. A lot of effort has been put in the theoretical investigation of the multivariate Padé approximation problem using different definitions (see Sections 3 and 7). The numerical implementation raises two delicate issues. First, there is the need to see the wood for the trees again: switching from one to many variables greatly increases the number of choices to be made on the way (see Sections 1 and 5). Second, there is the typical problem of breakdown when computing ratios of determinants: the added value of interval arithmetic combined with defect correction turns out to be significant (see Sections 2 and 4). In Section 6 these two problems are thoroughly illustrated and the interested reader is taken by the hand and guided through a typical computation session. On the way some open problems are indicated which motivate us to continue our research mainly in the area of gathering and offering more knowledge about the problem domain on one hand, and improving the arithmetic tools and numerical routines for a reliable computation of the approximants on the other hand.

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1. The Need for Knowledge in Multivariate Approximation

For many types of problems traditional libraries of numerical routines exist. As more algorithms become available to solve problems within a particular domain, these libraries grow larger and the need arises to augment them with rules to guide the user with the selection of an appropriate routine. To this end a number of knowledge-based environments for libraries of numerical routines have been developed [4, 3]. The need for "knowledge" or guidance in numerical routines also arises naturally in another context. Indeed, as the problems to be solved grow in complexity, which is often the case when one is dealing with multivariate problems, the options within

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a single algorithm increase and influence the final outcome. Therefore the amount of expertise available to help the user make the correct choices determines, for multivariate much more than for univariate approximation problems, the quality of the approximation. The transition from the univariate to the multivariate case greatly increases the number of choices to be made when constructing an approximant. We shall show by typical examples the crucial importance of basing such choices on symmetry information, pole and zero information, convergence results, covariance and invariance properties etc. These examples motivate more than enough the need for the inclusion of knowledge in software to approximate a multivariate function $f(x_1, \ldots, x_n)$.

Whether one considers multivariate rational approximants or multivariate splines to approximate a multivariate function $f(x_1, \ldots, x_n)$, all these approaches have one thing in common: the choices to be made when constructing the multivariate approximant (degrees of numerator and denominator, knot set ...) are much more complex than in the univariate case. Selecting an approximation strategy (splines, rational approximants, ...) is usually a clear cut choice and is determined by the nature of the problem. It becomes more difficult, especially for naive users, to decide which rational approximant or which spline function best approximates the function given.

Usually, within a chosen field, a sequence of approximants is constructed. The motivation for this is twofold. Either the user hopes that the sequence of approximants yields comparable numerical output, in which case no selection is needed and the different approximants "confirm" each other. Or the user expects improvement from the sequence of approximants because of some convergence properties. In the most general case, the user is faced with the problem of selecting one out of many approximants because the numerical output varies due to slightly different choices made when constructing the approximants. It is clear that a good choice of approximant should only be guided by valid arguments which reflect both knowledge about the given data and knowledge about the problem domain.

With respect to the latter, theorems about the convergence of sequences of approximants, about covariance and invariance properties and the like play an important role in providing guidance to compute good approximants. With respect to the former, any information concerning symmetry, pole and/or zero information of the function $f(x_1, \ldots, x_n)$ should be taken into account. In order to illustrate the above principles, we have developed a case study for multivariate Padé approximants.

2. The Need for Reliability in Scientific Computation

Several numerical methods require the computation of a ratio of determinants for their solution. Rational approximation, convergence acceleration, orthogonal polynomials, ... are just a few of these. Algorithms to compute such ratios of determinants are prone to breakdown and instability because of possible division by near-zero [2]. In this respect we investigate the added value of using interval arith-

metic combined with defect correction.

In the previous section we mentioned that when constructing a sequence of approximants, the numerical output may vary from one approximant to another. We can only make sure that this variation in output is indeed mainly due to the quality of the approximant if the algorithms to compute the respective approximants yield "guaranteed" results, i.e. enclosures in which the true result is enclosed. The most obvious way to obtain an inclusion of the true result is to apply the algorithm with all operations replaced by their corresponding interval operation. As has been shown in the literature, this simplistic approach may yield unrealisticly pessimistic bounds. It is this behaviour which has discredited interval arithmetic in the past.

To get around this problem, the idea of the E-method [29] has been developed. E-methods (E for Existence and Enclosure) are also called "self-validating" algorithms since they automatically verify the result of a numerical computation. The methods start with an approximation of the result which can be obtained by conventional numerical methods. Afterwards, the initial approximation is improved, usually by applying a fixed-point theorem implemented on the computer in interval arithmetic. It has been shown [29] that it is useful in this respect to evaluate scalar product expressions optimally. If the conditions to apply the fixed-point theorem are satisfied in floating-point interval arithmetic, then they are also satisfied in exact arithmetic. Indeed, let the interval extension of the iteration function f be denoted by F (mathematically defined and hence only computable in exact arithmetic with infinite precision) and let $\textcircled{F}$ be the implementation of F in floating-point interval arithmetic using finite precision, then

$$f(x) \in F(X) \subseteq \textcircled{F}(X)$$

always holds. Therefore $\textcircled{F}(X) \subseteq X$ implies $F(X) \subseteq X$ and the fixed-point theorem can be applied. When an enclosure of the result cannot be obtained an appropriate message is displayed. In no case an unreliable result is produced.

One of the problems which can easily be rewritten as a fixed-point problem is the solution of a linear system of equations $Ax = b$. We focus on this problem since we shall see in the following sections that there is a close link between solving a linear system of equations and computing a multivariate Padé approximant. Solving the system of equations $Ax = b$ is equivalent to finding a fixpoint of the iteration function $f(e)$ defined by

$$f(e) = R(b - A\tilde{x}) + (I - RA)e$$

with R a nonsingular matrix and $\tilde{x}$ an approximate solution of $Ax = b$. The fixpoint of $f(e)$ is the defect vector $e = \hat{x} - \tilde{x}$, where $\hat{x}$ is the exact solution of $Ax = b$. The following theorem [28] can be applied in computer interval arithmetic to obtain guaranteed bounds for the solution of the linear system of equations $Ax = b$.

THEOREM 1. *Let* $F(E) = R(b - A\tilde{x}) + (I - RA)E$ *be the interval extension of*

$f(e)$. *If for some interval vector* E

$$F(E) \subseteq \overset{\circ}{E}$$

holds, then the linear system $Ax = b$ *has one and only one solution* $\hat{x}$ *in* $\tilde{x} + \overset{\circ}{E}$, *where* $\overset{\circ}{E}$ *denotes the interior of the interval vector* E.

The algorithm which implements this theorem to solve a linear system of equations is given in pseudo-code in Appendix A and is referred to as LSS (Linear System Solver) [23, p. 179–181],[29]. It will turn out to play an important role in order to obtain guaranteed bounds in the computation of multivariate approximants.

3. The Problem Domain: Multivariate Padé Approximants

We restrict our description to the bivariate case, only for notational convenience, although we use the term multivariate in the text. Given a Taylor series expansion

$$f(x,y) = \sum_{(i,j)\in\mathbf{N}^2} c_{ij}(x-x_0)^i(y-y_0)^j$$

with

$$c_{ij} = \frac{1}{i!}\frac{1}{j!}\frac{\partial^{i+j} f}{\partial x^i \partial y^j}(x_0,y_0)$$

we compute a Padé approximant $p(x,y)/q(x,y)$ to $f(x,y)$ where the polynomials $p(x,y)$ and $q(x,y)$ are given by

$$p(x,y) = \sum_{(i,j)\in N} a_{ij}(x-x_0)^i(y-y_0)^j \qquad N \subset \mathbf{N}^2 \qquad \#N = n+1 \quad (1a)$$

$$q(x,y) = \sum_{(i,j)\in D} b_{ij}(x-x_0)^i(y-y_0)^j \qquad D \subset \mathbf{N}^2 \qquad \#D = m+1 \quad (1b)$$

and are determined by the following "accuracy through order" principle [12]:

$$(fq-p)(x,y) = \sum_{(i,j)\in\mathbf{N}^2\setminus I} d_{ij}(x-x_0)^i(y-y_0)^j \qquad (1c)$$
$$I \subset \mathbf{N}^2 \qquad \#I = n+m+1$$

where rules for choosing I appropriately are given below in (2). For the sake of simplicity we assume that $(x_0,y_0) = (0,0)$ in the sequel of the text unless otherwise specified.

The finite index sets N and D indicate the "degree" of $p(x,y)$ and $q(x,y)$. We shall also refer to them as "degree sets". It is among others possible to let $p(x,y)$

and $q(x, y)$ satisfy (1) if, in analogy with the univariate case, the index set $I \subset \mathbf{N}^2$ is chosen such that

$$N \subseteq I \tag{2a}$$

$$\#(I \backslash N) = m = \#D - 1 \tag{2b}$$

$$I \quad \text{satisfies the inclusion property} \tag{2c}$$

meaning that when a point belongs to the index set I, then the rectangle of points emanating from the origin with the given point as its furthermost corner is a subset of I.

Condition (2a) enables us to split the system of equations

$$d_{ij} = 0 \qquad (i, j) \in I$$

in an inhomogeneous part defining the numerator coefficients

$$\sum_{\mu=0}^{i} \sum_{\nu=0}^{j} c_{\mu\nu} b_{i-\mu, j-\nu} = a_{ij} \qquad (i, j) \in N \tag{3a}$$

and a homogeneous part defining the denominator coefficients

$$\sum_{\mu=0}^{i} \sum_{\nu=0}^{j} c_{\mu\nu} b_{i-\mu, j-\nu} = 0 \qquad (i, j) \in I \backslash N \tag{3b}$$

By convention

$$b_{kl} = 0 \quad \text{if} \quad (k, l) \notin D$$

Condition (2b) guarantees the existence of a nontrivial denominator $q(x, y)$ because the homogeneous system has one equation less than the number of unknowns and so one unknown coefficient can be chosen freely.

Condition (2c) finally takes care of the Padé approximation property, namely when $q(x_0, y_0) \neq 0$ then

$$(f - \frac{p}{q})(x, y) = \sum_{(i,j) \in \mathbf{N}^2 \backslash I} e_{ij} x^i y^j$$

For more information we refer to [11, p. 22]. We denote a solution $p(x, y)/q(x, y)$ of this general order multivariate Padé approximation problem (1) by $[N/D]_I$.

4. Techniques for Their Computation

In order to describe the different algorithms for the computation of multivariate Padé approximants we first order the Padé approximants in a table, where, when walking along columns the numerator degree set increases, while when walking along rows the denominator degree set increases. Since, unlike in the univariate case, the way to increase a degree set is not unique, one has to prescribe which is the next term to be added. Let us therefore introduce enumerations r_N and r_D for the elements of the sets N and D:

$$r_N : N \longrightarrow \mathbf{N} : (i,j) \longrightarrow r_N(i,j)$$
$$r_D : D \longrightarrow \mathbf{N} : (i,j) \longrightarrow r_D(i,j)$$

We assume throughout the text that the numberings are such that

$$i \leq k \text{ and } j \leq \ell \Rightarrow r(i,j) \leq r(k,\ell)$$

With this numbering, we can set up descending chains of degree sets, defining bivariate polynomials of "lower degree"

$$\begin{aligned} N = N_n \supset \ldots \supset N_k = \{(i_0,j_0),\ldots,(i_k,j_k)\} \supset \ldots \\ \supset N_0 = \{(i_0,j_0)\} \qquad k = 0,\ldots,n \end{aligned} \tag{4a}$$

$$\begin{aligned} D = D_m \supset \ldots \supset D_\ell = \{(d_0,e_0),\ldots,(d_\ell,e_\ell)\} \supset \ldots \\ \supset D_0 = \{(d_0,e_0)\} \qquad \ell = 0,\ldots,m \end{aligned} \tag{4b}$$

where the bivariate Padé approximants of "lower order"

$$[N_k/D_\ell]_{I_{k+\ell}}$$

satisfy the subset $I_{k+\ell}$ of the first $k+\ell+1$ approximation conditions of I. It is therefore also necessary to introduce a numbering r_I for the set I, taking into account that condition (2a) remains satisfied for the intermediate Padé approximants:

$$\begin{aligned} I = I_{n+m} \supset \ldots \supset I_{k+\ell} = N_k \cup \{(i_{k+1},j_{k+1}),\ldots,(i_{k+\ell},j_{k+\ell})\} \supset \ldots \\ \supset I_0 = N_0 \qquad k+\ell = 0,\ldots,n+m \end{aligned} \tag{4c}$$

Once the numberings r_N, r_D and r_I are chosen, we can compute the following entries in a "table" of multivariate Padé approximants:

$$\begin{array}{ccc} [N_0/D_0]_{I_0} & \ldots & [N_0/D_m]_{I_m} \\ \vdots & & \vdots \\ [N_n/D_0]_{I_n} & \ldots & [N_n/D_m]_{I_{n+m}} \end{array} \tag{5}$$

In order to compute the Padé approximants in the table, different techniques have been developed. Let us first recall the link between the computation of Padé approximants and the solution of linear systems of equations. Clearly, solving the system of equations (3) yields the coefficients of the Padé approximant. From (3) the following explicit determinant representation for the $[N/D]_I = [N_n/D_m]_{I_{n+m}}$ Padé approximant can also be deduced:

$$\frac{p(x,y)}{q(x,y)} =$$

$$\frac{\begin{vmatrix} \sum\limits_{(i,j)\in N_n} c_{i-d_0,j-e_0} x^{i-d_0} y^{j-e_0} & \cdots & \sum\limits_{(i,j)\in N_n} c_{i-d_m,j-e_m} x^{i-d_m} y^{j-e_m} \\ c_{i_{n+1}-d_0,j_{n+1}-e_0} x^{i_{n+1}-d_0} y^{j_{n+1}-e_0} & \cdots & c_{i_{n+1}-d_m,j_{n+1}-e_m} x^{i_{n+1}-d_m} y^{j_{n+1}-e_m} \\ \vdots & & \vdots \\ c_{i_{n+m}-d_0,j_{n+m}-e_0} x^{i_{n+m}-d_0} y^{j_{n+m}-e_0} & \cdots & c_{i_{n+m}-d_m,j_{n+m}-e_m} x^{i_{n+m}-d_m} y^{j_{n+m}-e_m} \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ c_{i_{n+1}-d_0,j_{n+1}-e_0} x^{i_{n+1}-d_0} y^{j_{n+1}-e_0} & \cdots & c_{i_{n+1}-d_m,j_{n+1}-e_m} x^{i_{n+1}-d_m} y^{j_{n+1}-e_m} \\ \vdots & & \vdots \\ c_{i_{n+m}-d_0,j_{n+m}-e_0} x^{i_{n+m}-d_0} y^{j_{n+m}-e_0} & \cdots & c_{i_{n+m}-d_m,j_{n+m}-e_m} x^{i_{n+m}-d_m} y^{j_{n+m}-e_m} \end{vmatrix}} \tag{6}$$

The representation (6) implies that the value of the Padé approximant in (x, y) can be computed as the first unknown of the system of linear equations $A\,x = b$ where

$$A = \begin{pmatrix} 1 & \cdots & 1 \\ c_{i_{n+1}-d_0,j_{n+1}-e_0} x^{i_{n+1}-d_0} y^{j_{n+1}-e_0} & \cdots & c_{i_{n+1}-d_m,j_{n+1}-e_m} x^{i_{n+1}-d_m} y^{j_{n+1}-e_m} \\ \vdots & & \vdots \\ c_{i_{n+m}-d_0,j_{n+m}-e_0} x^{i_{n+m}-d_0} y^{j_{n+m}-e_0} & \cdots & c_{i_{n+m}-d_m,j_{n+m}-e_m} x^{i_{n+m}-d_m} y^{j_{n+m}-e_m} \end{pmatrix}^T \tag{7a}$$

and

$$b = \left(\sum_{(i,j)\in N_n} c_{i-d_0,j-e_0} x^{i-d_0} y^{j-e_0} \quad \cdots \quad \sum_{(i,j)\in N_n} c_{i-d_m,j-e_m} x^{i-d_m} y^{j-e_m} \right)^T \tag{7b}$$

The determinant representation (6) of the Padé approximant also lends itself to recursive computation using the E-algorithm [13]. If we denote

$$[N_k/D_\ell]_{I_{k+\ell}} = E_\ell^{(k)} \qquad k = 0, \ldots, n \qquad \ell = 0, \ldots, m$$

then for $r = 0, \ldots, n+m$

$$\begin{aligned}
E_0^{(r)} &= \sum_{(i,j)\in N_r} c_{i-d_0,j-e_0} x^{i-d_0} y^{j-e_0} \\
g_{0,s}^{(r)} &= \sum_{(i,j)\in N_r} c_{i-d_s,j-e_s} x^{i-d_s} y^{j-e_s} - \\
&\qquad \sum_{(i,j)\in N_r} c_{i-d_{s-1},j-e_{s-1}} x^{i-d_{s-1}} y^{j-e_{s-1}} \qquad s = 1, ..., m \\
g_{h,s}^{(r)} &= \frac{g_{h-1,s}^{(r)} g_{h-1,h}^{(r+1)} - g_{h-1,s}^{(r+1)} g_{h-1,h}^{(r)}}{g_{h-1,h}^{(r+1)} - g_{h-1,h}^{(r)}} \qquad h = 1, \ldots, s-1 \\
E_s^{(r)} &= \frac{E_{s-1}^{(r)} g_{s-1,s}^{(r+1)} - E_{s-1}^{(r+1)} g_{s-1,s}^{(r)}}{g_{s-1,s}^{(r+1)} - g_{s-1,s}^{(r)}} \qquad s = 1, 2, ..., n
\end{aligned} \tag{8}$$

The multivariate Padé-approximants $[N_n/D_m]_{I_{n+m}}$ with $n \geq m$ can also be written in continued fraction form [14]

$$\begin{aligned}
[N_n/D_m]_{I_{n+m}} = \; & [N_{n-m}/D_0]_{I_{n-m}} \\
& + \cfrac{c_{i_{n-m+1}-d_0, j_{n-m+1}-e_0} x^{i_{n-m+1}-d_0} y^{j_{n-m+1}-e_0}}{1} \\
& + \cfrac{-q_1^{(n-m+1)}(x,y)}{1+q_1^{(n-m+1)}(x,y)} + \cfrac{-e_1^{(n-m+1)}(x,y)}{1+e_1^{(n-m+1)}(x,y)} \\
& + \cfrac{-q_2^{(n-m+1)}(x,y)}{1+q_2^{(n-m+1)}(x,y)} + \cfrac{-e_2^{(n-m+1)}(x,y)}{1+e_2^{(n-m+1)}(x,y)} \\
& + \ldots + \cfrac{-q_m^{(n-m+1)}(x,y)}{1+q_m^{(n-m+1)}(x,y)}
\end{aligned} \tag{9}$$

where the coefficients of the continued fraction are computed via a multivariate qd-like scheme. Computing the same g-values as in the E-algorithm, we have

$$q_1^{(n-m+1)}(x,y) = -\frac{c_{i_{n-m+2}-d_0,j_{n-m+2}-e_0}x^{i_{n-m+2}-d_0}y^{j_{n-m+2}-e_0}}{c_{i_{n-m+1}-d_0,j_{n-m+1}-e_0}x^{i_{n-m+1}-d_0}y^{j_{n-m+1}-e_0}} \times \frac{g_{0,1}^{(n-m+1)}}{g_{0,1}^{(n-m+2)} - g_{0,1}^{(n-m+1)}}$$

$$q_s^{(n-m+1)}(x,y) = q_{s-1}^{(n-m+2)} \frac{e_{s-1}^{(n-m+2)}}{e_{s-1}^{(n-m+1)}} \frac{g_{s-2,s-1}^{(n-m+s)} - g_{s-2,s-1}^{(n-m+s-1)}}{g_{s-2,s-1}^{(n-m+s-1)}} \times \frac{g_{s-1,s}^{(n-m+s)}}{g_{s-1,s}^{(n-m+s+1)} - g_{s-1,s}^{(n-m+s)}} \quad s = 2,\ldots,m \tag{10}$$

$$e_s^{(n-m+1)}(x,y) = -\frac{g_{s-1,s}^{(n-m+s+1)} - g_{s-1,s}^{(n-m+s)}}{g_{s-1,s}^{(n-m+s)}} \left(q_s^{(n-m+2)} + 1\right) - 1 \quad s = 1,\ldots,m-1$$

The convergents of the continued fraction (9) are successive elements on staircases in the table of multivariate Padé approximants.

5. Knowledge about Their Convergence Behaviour

When approximating a multivariate function, one usually constructs a sequence of approximants $S = \{r_0, r_1, r_2, \ldots,\}$ from which one approximant is then selected. When the r_n are multivariate Padé approximants the sequence S may be a row, a column, a diagonal, a staircase, ... in the Padé table. Because of well-known convergence theorems for Padé approximants, it may turn out that certain sequences of approximants are to be preferred over others. Let us first recall some of the results on the convergence of univariate Padé approximants which have been or are now being investigated for multivariate Padé approximants. We denote by $[k/\ell]_{k+\ell}$ the Padé approximant of degree k in the numerator and degree ℓ in the denominator for a univariate function f.

First we take $r_n(x) = [n/0]_n(x)$, the partial sums of the Taylor series expansion for $f(x)$. The following result is obvious.

THEOREM 2. *If f is analytic in $B(0,r)$ with $r > 0$, then $S = \{[n/0]_n\}_{n\in\mathbf{N}}$ converges uniformly to f in $B(0,r)$.*

Next take $r_n(x) = [n/1]_{n+1}(x)$ from the first column in the Padé table for f. It is possible to construct functions f that are analytic in the whole complex plane but for which the poles of the $[n/1]_{n+1}$ Padé approximant are a dense subset of $\mathbf{C}$ [27, p. 158]. So in general S will not converge. But the following theorem can be proved [1].

THEOREM 3. *If f is analytic in $B(0,r)$ with $r > 0$, then an infinite subsequence of $\{[n/1]_{n+1}\}_{n\in\mathbf{N}}$ exists which converges uniformly to f in $B(0,r)$.*

For meromorphic functions f it is also possible to prove the convergence of a particular column in the Padé table [20].

THEOREM 4. *If f is analytic in $B(0,r)$ except in the distinct poles $w_1,\ldots,w_k$ of f with total multiplicity m and with*

$$0 < |w_1| \leq |w_2| \leq \ldots \leq |w_k| < R$$

then $\{[n/m]_{n+m}\}_{n\in\mathbf{N}}$ converges uniformly to f in $B(0,r) \setminus \{w_1,\ldots,w_k\}$.

Also for meromorphic functions another kind of convergence can be proved for the diagonal approximants. It is called convergence in measure [26].

THEOREM 5. *Let f be meromorphic and let G be a closed and bounded subset of $\mathbf{C}$. For every $\epsilon > 0$ and $\delta > 0$ there exists an integer k such that for $n > k$ we have*

$$|[n/n]_{2n}(x) - f(x)| < \epsilon \qquad x \in G_n$$

where G_n is a subset of G such that the measure of $G \setminus G_n$ is less than δ.

So far for the univariate case. For the multivariate case a generalization of Theorem 2 clearly holds. As for Theorem 3, remember that the first column in the multivariate Padé table has denominator degree set $D = \{(d_0,e_0),(d_1,e_1)\} \subset \mathbf{N}^2$. However this set is not uniquely determined and therefore no straightforward meaningful equivalent of Theorem 3 should be proved for the multivariate case. The analogue of the de Montessus de Ballore's theorem for multivariate Padé approximants was proved in [15, 16] and is given below.

THEOREM 6. *Let $f(x,y)$ be a multivariate function which is meromorphic in the polydisc $B(0;R_1,R_2) = \{(x,y) : |x| < R_1, |y| < R_2\}$ meaning that there exists a polynomial*

$$R_m(x,y) = \sum_{(d,e)\in D\subseteq\mathbf{N}^2} r_{de}x^d y^e = \sum_{i=0}^{m} r_{d_ie_i}x^{d_i}y^{e_i}$$

such that $(fR_m)(x,y)$ is analytic in the polydisc above. Further, we assume that $R_m(0,0) \neq 0$ so that necessarily $(0,0) \in D$. Then the $[N/D]_I = (p/q)(x,y)$

Padé approximant with D fixed as given above and N and I growing towards $\mathbf{N}^2$, converges to $f(x,y)$ uniformly on compact subsets of

$$\{(x,y) : |x| < R_1, |y| < R_2, R_m(x,y) \neq 0\}$$

and its denominator

$$q(x,y) = \sum_{i=0}^{m} b_{d_i e_i} x^{d_i} y^{e_i}$$

converges to $R_m(x,y)$ under the following conditions for N and I. The index sets N and I should grow towards $\mathbf{N}^2$ along the m^{th} column in the Padé table in such a way that $\max\{s \mid \forall t, 0 \leq t \leq s \ : \ (t, s-t) \in I\} \to \infty$ *and* $\max\{s \mid \exists t, 0 \leq t \leq s \ : \ (t, s-t) \in N * D\} \to \infty$ *where* $N * D = \{(i+k, j+\ell) | (i,j) \in N, (k,\ell) \in D\}$.

If we denote by T_s the isosceles triangle in $\mathbf{N}^2$ with top in $(0,0)$ and base along the s^{th} upward sloping diagonal:

$$T_s = \{(i,j) \in \mathbf{N}^2 \mid 0 \leq i + j \leq s\}$$

then the conditions on I and N in Theorem 6 say that the largest set T_{s_1} which is contained in I and the smallest set T_{s_2} which contains $N * D$ must both tend to $\mathbf{N}^2$ as the sets I and N grow along a column in the multivariate Padé table.

Finally, the generalization of Theorem 5 on the convergence in measure of diagonal multivariate Padé approximants for some special choice of N, D and I as discussed in Section 7, is currently under investigation.

6. Numerical Case Study

In this section we aim at illustrating via a numerical example and via the computation of multivariate Padé approximants how knowledge and reliability are needed in order to obtain correct approximation results. It is well-known that one can obtain both good and bad approximation results when computing an approximant. However, the bad results are not necessarily due to the approximation technique but sometimes rather to a lack of knowledge about the problem to make the right choices when constructing an approximant. These remarks also apply to the domain of multivariate Padé approximation.

The example we use is the Beta function, which is defined by

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$$

where Γ is the Gamma function. The Beta function is meromorphic in $\mathbf{C}^2$ with polar singularities occurring at $x = -k$ and $y = -k$ for $k = 0, 1, 2, \ldots$ and zeros at $y = -x - k$ for $k = 0, 1, 2, \ldots$ By means of the recurrence formulas

$$\Gamma(x+1) = x\Gamma(x)$$
$$\Gamma(y+1) = y\Gamma(y)$$

for the Gamma function, we can write

$$B(x,y) = \frac{1+(x-1)(y-1)f(x-1,y-1)}{xy} \tag{11a}$$

Writing the Beta function as above extracts in a simple way the poles $x = 0$ and $y = 0$. We are hence going to compute approximants for the Beta function by constructing Padé approximants $[N/D]_I(x,y)$ for the function $f(x-1,y-1)$ and compare the exact value $B(u_i,v_j)$ with the value

$$\frac{1+(u_i-1)(v_j-1)[N/D]_I(u_i,v_j)}{u_i v_j} \tag{11b}$$

in different points (u_i,v_j). In order to do so, we need the function $f(x-1,y-1)$ in the form of a Taylor series expansion. Our data are the coefficients c_{ij} of the Taylor series expansion for $f(x-1,y-1)$ around $(1,1)$ with $0 \leq i+j \leq 32$. Hence the index sets $I_{k+\ell}$ satisfy at each moment

$$I_{k+\ell} \subseteq \{(i,j) \mid 0 \leq i+j \leq 32\} \qquad \#I_{k+\ell} \leq 561$$

With the given data different Padé approximants can be constructed, namely the

$$[N_k/D_\ell]_{I_{k+\ell}} \qquad 0 \leq k+\ell \leq 560$$

Let r_I and r_N be the following numberings along upward sloping diagonals in $\mathbf{N}^2$:

$(0,0)$	$(1,0)$	$(0,1)$	$(2,0)$	$(1,1)$	$(0,2)$	$(3,0)$	$(2,1)$	$(1,2)$	$\ldots$
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	
0	1	2	3	4	5	6	7	8	$\ldots$

(12a)

or, equivalently

$$r_I(i,j) = r_N(i,j) = \frac{(i+j)(i+j+1)}{2} + j$$

and let r_D be the following numbering along squares in $\mathbf{N}^2$:

$(0,0)$	$(1,0)$	$(0,1)$	$(1,1)$	$(2,0)$	$(2,1)$	$(0,2)$	$(1,2)$	$(2,2)$	$\ldots$
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	
0	1	2	3	4	5	6	7	8	$\ldots$

(12b)

The importance of generating square subsets D_ℓ for $\ell = 0, 3, 8, \ldots$ by using the numbering (12b) will become apparent further on.

At first we consider the Padé approximants $[N_k/D_\ell]_{I_{k+\ell}}$ where $k \leq 119$ and $\ell \leq 3$. With the numberings r_I, r_N and r_D given by (12) we have

$$N_{119} = \{(i,j) \mid 0 \leq i+j \leq 14\}$$

and

$$\begin{aligned} D_0 &= \{(0,0)\} \\ D_2 &= \{(0,0),(1,0),(0,1)\} \\ D_3 &= \{(0,0),(1,0),(0,1),(1,1)\} \end{aligned} \tag{13}$$

The computation by the E-algorithm of the Padé approximants for $f(x-1, y-1)$ followed by the evaluation of (11b), both in $(-0.75, -0.75)$, yields Table 1.

Note that there are big discrepancies for "nearby" approximants, i.e. approximants of which the degree sets differ in only one term like $E_2^{(103)}$ and $E_3^{(103)}$ or $E_3^{(105)}$ and $E_3^{(106)}$. The question now arises whether these discrepancies are due to numerical instability of the E-algorithm (note that the E-algorithm is prone to near-breakdown) or to data contamination. If this is not the case there is clearly need of knowledge to choose the approximant which really approximates the Beta function in $(-0.75, -0.75)$. These issues will be addressed in the next sections.

6.1. RELIABLE RESULTS?

In order to check whether or not the discrepancies are due to numerical instability of the E-algorithm or are a consequence of input perturbation, different ways can be walked. In a first approach, we reran the E-algorithm in interval mode so as to obtain guaranteed bounds for the results. However, as has already often been pointed out in the literature, the intervals tend to grow (too) quickly during the course of the computation. In the E-algorithm in particular, the intervals $g_{s-1,s}^{(r+1)} - g_{s-1,s}^{(r)}$ appearing in the denominator of (8) soon ($r = 110, s = 3$) grow so large that they contain 0, even though the floating point value of the expression is in many cases larger than 1, causing a breakdown of the algorithm. Another approach is to compute the Padé approximants via another algorithm. As already pointed out, the multivariate qd-like algorithm (10) also relies heavily on the computation of the g-values and hence similar output can be expected.

Last but not least however, we recall the important link between the computation of Padé approximants and the solution of linear systems of equations. Obtaining reliable and accurate results for the solution of a linear system of equations, even if that linear system is ill-conditioned, has been investigated thoroughly. As mentioned in Section 2 we make use of the LSS technique which implements defect correction in computer interval arithmetic using the exact scalar product to solve the system

n \ m	0	2	3
95	6.272469539927058	6.382241356832849	6.252199337861037
96	6.272481219879103	6.373969995330925	6.252199326007094
97	6.272487831740126	6.382244442674818	6.266577260911057
98	6.272494443601187	6.410072833517622	6.300404767334740
99	6.272506123553238	6.469560908765764	6.369481476489413
100	6.272544497731672	6.597917327186983	9.722877909033864
101	6.272810203348119	9.737548612905988	9.895775024125525
102	6.277863394645692	9.847326401470260	9.312348514619972
103	6.757612224375486	5.373819134560423	9.420269191090856
104	6.517174482717973	9.879269550748257	9.920113846171462
105	6.306954585440170	9.801348477243014	9.793178514188524
106	6.726741855333899	7.021564358750562	6.826017824698794
107	6.729671095099285	6.906974546767763	6.761484996863231
108	6.729784277460005	6.852286196295363	6.727815545486309
109	6.729796844258718	6.824588041048912	6.710913104188903
110	6.729799835419403	6.812657490354739	6.705716580531475
111	6.729801157749264	6.812657738724513	6.710913100069901
112	6.729802171934143	6.824588676978205	6.727815664029961
113	6.729803494264011	6.852286709821294	6.761485208089148
114	6.729806485424670	6.906972882457715	6.826017206347385
115	6.729819052223378	7.021547253788186	9.792927727303981
116	6.729932234584101	9.799275262541185	9.891548307005404
117	6.732861474349487	9.864013647323537	9.553039471914062
118	7.152648744243218	5.949314052499588	9.619286021637370
119	6.942428846965417	9.882493034609045	9.905525832249440

Table 1

n \ m	2	3
100	[6.5979172, 6.5979175]	[9.722877904, 9.722877914]
101	[9.737548608, 9.737548618]	[9.89577500, 9.89577505]
102	[9.84732638, 9.84732643]	[9.3123483, 9.3123487]
103	[5.373819134, 5.373819135]	[9.4202690, 9.4202694]
104	[9.87926953, 9.87926957]	[9.92011383, 9.92011387]
105	[9.801348474, 9.801348481]	[9.793178510, 9.793178518]
106	[7.0215641, 7.0215646]	[6.826016, 6.826020]
107	[6.906973, 6.906976]	[6.76147, 6.76150]
108	[6.852282, 6.852290]	[6.72778, 6.72785]
109	[6.82458, 6.82460]	[6.7108, 6.7110]
110	[6.812654, 6.812661]	[6.7056, 6.7059]

Table 2

of equations (7). The output of the LSS algorithm for some of the floating-point results of Table 1 is given in Table 2.

Having used interval input and interval arithmetic we know that the above bounds for the output are reliable. Hence we can conclude from Table 2 that the discrepancies between different Padé approximants can, in this numerical example, not be attributed to numerical instability of the algorithm used to compute the Padé approximants, because all rounding errors are taken into account. From the fact that we used interval input to generate Table 2, we can also conclude that the discrepancies cannot be attributed to the effect of poor data, poor meaning that some data have few significant digits. Moreover, this illustrates that tools for reliable computation are necessary to answer the first question raised. Let us now compare the computed value of the Padé approximants in $(-0.75, -0.75)$ with the exact value of the Beta function in that point

$$B(-0.75, -0.75) = 9.88839829\ldots$$

We will indicate in the next section how good numerical results can be computed if knowledge about the problem (not about the result !) is available. This knowledge can be obtained for instance by deciphering the power series expansion.

We also note that the problem of constructing Padé approximants for the bivariate function $f(x-1, y-1)$ is a tough one. Indeed, the coefficients c_{ij} in the Taylor series expansion of $f(x-1, y-1)$ range between $\pm 10^{-1}$ and $\pm 10^{-19}$. It is difficult to solve a problem where the data vary so much in magnitude without losing significant digits. A similar remark can be made for the coefficients in the Taylor series expansion of the Beta function around $(1, 1)$. So the problem does not come from rewriting the Beta function in its form (11a). After noting the huge variation in size of the coefficients, one may wonder how many significant digits the small order coefficients still have. This type of information signals the user for the accuracy that can be expected from the final outcome. If the input contains data having only few significant digits, then one cannot expect in general that the approximant estimates the function with full double precision accuracy. To obtain information on the number of significant digits of our input data, we have computed the Taylor coefficients c_{ij} of the Taylor series expansion for $f(x-1, y-1)$ around $(1, 1)$ in interval mode. The results of this computation are given in Table 3.

We recall that the numbering r_I determines the order in which the data necessary to compute an approximant are used. If not all data c_{ij} have the same number of significant digits, it is appropriate to choose r_I in such a way that data with the least number of significant digits are used last. In this way the largest data perturbations have least effect and the output results are more stable. To illustrate this, we choose numberings $r_N = r_I$ along prongs in $\mathbf{N}^2$ as follows:

$$\begin{array}{ccccccccccc} (0,0) & (1,0) & (0,1) & \ldots & (32,0) & (0,32) & (1,1) & \ldots & (31,1) & (1,31) & \ldots \\ \downarrow & \downarrow & \downarrow & & \downarrow & \downarrow & \downarrow & & \downarrow & \downarrow & \\ 0 & 1 & 2 & \ldots & 63 & 64 & 65 & \ldots & 124 & 125 & \ldots \end{array}$$

i	j	c_{ij}
0	5	$[8.349277381922821E-3, 8.349277381922831E-3]$
0	6	$[-4.077356197944342E-3, -4.077356197944336E-3]$
0	22	$[-5.96081890512602E-8, -5.96081890512599E-8]$
0	23	$[2.98035035146499E-8, 2.98035035146501E-8]$
1	5	$[7.76445005366089E-3, 7.76445005366093E-3]$
1	6	$[-3.89545972581657E-3, -3.89545972581654E-3]$
1	22	$[-5.9604642984845E-8, -5.9604642984842E-8]$
1	23	$[2.9802321940708E-8, 2.9802321940710E-8]$
6	5	$[-7.703022618E-8, -7.703022606E-8]$
6	6	$[7.7651340E-9, 7.7651343E-9]$
6	22	$[5.4E-18, 7.1E-18]$
6	23	$[-2.65E-16, -2.63E-16]$

Table 3

As can be deduced from Table 3 and in contrast with r_I given by (12a), this numbering places input coefficients c_{ij} with few significant digits at the end of the input list. With this numbering for r_I and r_N, we compute multivariate Padé approximants $[N_k/D_3]_{I_{k+3}}$ in $(-0.75, -0.75)$, where D_3 is given by (13). The output is given in Table 4.

We have displayed just a few approximants which are representative for the entire sequence $[N_k/D_3]_{I_{k+3}}$. It is clear that with these data the numberings along prongs in $\mathbf{N}^2$ deliver more consistent output than the numberings along upward sloping diagonals.

6.2. KNOWLEDGE ABOUT THE PROBLEM DOMAIN!

A closer look at the approximation problem described above immediately reveals that the Beta function is a symmetric function. Therefore it seems appropriate that we only consider symmetric approximants, i.e. approximants for which the numerator set N_k, the denominator set D_ℓ and the index set $I_{k+\ell}$ are symmetric. In our example the considered denominators D_0, D_2 and D_3 are symmetric. With the numbering (12), the numerators and the index set can not both be symmetric at the same time, but as can be seen from Table 1 the approximants with either a symmetric numerator set N_k or a symmetric equation set $I_{k+\ell}$ are clearly much better approximants. Note for instance the difference between $[N_{103}/D_2]_{I_{105}}$ (non-symmetric numerator and non-symmetric equation set) and $[N_{102}, D_2]_{I_{104}}$ (symmetric equa-

n \ m	3
126	[9.6518761990, 9.6518761998]
136	[8.471761049, 8.471761054]
146	[8.36986616, 8.36986627]
156	[8.348959, 8.348962]
166	[8.34414, 8.34419]
176	[8.3423, 8.3431]
186	[9.6183984852, 9.6183984859]
196	[9.61703623, 9.61703631]
206	[9.620424, 9.620439]
216	[9.621, 9.623]
226	[9.585, 9.599]
236	[9.64627157, 9.64627160]
246	[9.66770, 9.66774]
256	[9.67, 9.69]
276	[9.59, 9.64]
286	[9.643717, 9.643720]
296	[9.658, 9.666]
336	[9.5, 9.8]
366	[9.50, 9.58]

Table 4

tion set) and $[N_{104}, D_2]_{I_{106}}$ (symmetric numerator degree set). Indeed,

$$N_{104} = I_{104} = \{(i,j) \mid 0 \leq i+j \leq 13\}$$

It is clear that since the numberings r_I, r_N and r_D can be chosen freely by the user of the algorithm, other numberings than (12) can be used to obtain that N_k, D_ℓ and $I_{k+\ell}$ are all symmetric simultaneously. For conciseness we do not introduce yet other numberings r_I and r_N to illustrate this. It should be noted, however, that in the example above where r_I and r_N are numberings along prongs in $\mathbf{N}^2$, all the Padé approximants $[N_k/D_\ell]_{I_{k+\ell}}$ always have either a symmetric numerator set N_k or a symmetric equation set $I_{k+\ell}$.

The power of multivariate Padé approximation as introduced in [25, 12, 19] and used here to approximate the function $f(x-1, y-1)$, and hence also the Beta function, comes among others from the fact that there is total freedom in the choice of numerator and denominator degree sets. That a general choice is permissible becomes even more important when one wants to take into account pole information of the function to be approximated. Indeed, recall the multivariate de Montessus de Ballore Theorem 6 given in Section 5. The function $f(x-1, y-1)$ we are approximating has poles at

$$x = -k \quad \text{and} \quad y = -k \quad \text{for } k = 1, 2, \ldots$$

n \ m	0	2	3
400	141.6317455753568	130.2516228400785	130.4381628812514
401	141.6317456268321	155.8049201484003	−28.82052731325514
402	141.6317460053908	−28.82044959055106	−28.77703154424141
403	141.6321797473016	−28.78547705882433	−28.59705613733203
404	153.9484660939392	124.7621958460614	−28.65841612339194
405	147.7902747247583	−28.77625645195215	−28.77097654242645
406	141.1702362710272	−28.79900813729537	−28.79904919517655
407	154.4102441058581	167.9417387065251	154.5832176120316
408	154.4105549201058	154.6136125842232	154.8129856867255
409	154.4105551178835	154.8529645194832	152.6741055590067
410	154.4105551188334	169.2378706038586	149.0557182929770
411	154.4105551260009	162.6060514312578	132.7615835782946
412	154.4105551705808	161.1981896760531	130.9724553145543
413	154.4105553480299	160.1507914116921	131.0964837093944

Table 5

If Theorem 6 is to be applied to the function $f(x-1, y-1)$, one needs to look at Padé approximants whose denominator polynomials are of the form

$$(x+1)(x+2)\dots(x+\ell_1)(y+1)(y+2)\dots(y+\ell_2)$$

in other words, denominator polynomials whose degree set is given by

$$D_\ell = \{(i,j) \mid 0 \le i \le \ell_1, 0 \le j \le \ell_2\} \qquad \ell + 1 = (\ell_1 + 1)(\ell_2 + 1) \quad (14)$$

The set D_3 given by (13) corresponds to $\ell_1 = \ell_2 = 1$ and hence the column $[N_k/D_3]_{I_{k+3}}$ converges uniformly on compact subsets of

$$\{(x,y) : x > -2, y > -2, (x+1)(y+1) \neq 0\}$$

If we look at the output given in Table 1, we indeed see a difference between the behaviour of the $[N_k/D_2]$ and the $[N_k/D_3]$ approximants. The latter tend to jump around less than the former. Similar results can be observed when we look at the Padé approximants $[N_k/D_\ell]_{I_{k+\ell}}$ where $k \le 413$ and $\ell \le 3$, again with r_I, r_N and r_D defined by (12) but now in $(-1.15, -1.15)$. The results are given in Table 5. Note that $B(-1.15, -1.15) = -28.7414305\dots$.

We remark that $(-1.15, -1.15)$ is outside the region of convergence of the Taylor series for $f(x-1, y-1)$ as it is across the first natural boundary $x = -1, y = -1$. The importance of Theorem 6, hence also lies in the fact that the region of convergence is enlarged when Padé approximants are used. According to Theorem 6 the next column which converges is the column for which the denominator degree set satisfies (14) with $\ell_1 = \ell_2 = 2$. Remember from the univariate case [22, p. 641-643] that poles of equidistant modulus cannot be separated in the formulation of

the de Montessus de Ballore theorem. For more details with respect to this in the multivariate case we refer to [18]. Because the pole curves of the function $f(x-1, y-1)$ appear in pairs equidistant from the origin, it is meaningless to consider columns for which in (14) $\ell_1 \neq \ell_2$.

6.3. CORRECT APPROACH

From all the above it is clear that a user who is well-informed about algorithms and convergence theorems for multivariate Padé approximants would, when approximating the Beta function in $(-0.75, -0.75)$ or $(-1.15, -1.15)$, immediately choose a symmetric approximant with denominator degree D_3 given by (13) and perform the computations in interval arithmetic with defect correction. This correct approach generates Table 6 in which only those approximants $[N_k/D_3]_{I_{k+3}}$ with either a symmetric numerator degree set N_k or a symmetric equation set I_{k+3} are displayed. In other words,

$$N_k = \{(i,j) \mid 0 \leq i+j \leq s\} \qquad \#N_k = k+1 = \frac{(s+1)(s+2)}{2}$$
$$s = 1, 2, \ldots$$

or

$$I_{k+3} = \{(i,j) \mid 0 \leq i+j \leq s\} \qquad \#I_{k+3} = k+4 = \frac{(s+1)(s+2)}{2}$$
$$s = 1, 2, \ldots$$

The interval output in Table 6 is computed by solving the linear system of equations (7) with LSS. Using LSS has the advantage that only the significant digits of the output are displayed whereas other algorithms just dump the output of the (double precision) computations and the user has no clue as to which output digits are contaminated and which are not.

The message implicitly contained in Table 6 is the following. The increase in complexity when going from univariate to multivariate problems should not seduce a user dealing with a multivariate problem to compute garbage. Unuseful output is not to be blamed on the approximation method but for instance on the fact that the "degree" of a multivariate polynomial is no longer uniquely defined. For multivariate Padé approximants the notion of "degree" plays an essential role and it should be defined carefully depending on the situation. For example, when approximating the Beta function, the notion of "degree" is defined differently for the numerator and the denominator polynomial. For reasons which we have explained above, only degrees corresponding to square degree sets in $\mathbf{N}^2$ are to be considered for the denominator polynomial while for the numerator polynomial any degree corresponding to a symmetric degree set in $\mathbf{N}^2$ can be considered. The non-uniqueness of the multivariate notion of "degree" has been the basis for the many

n (3)	$B(-0.75,-0.75) = 9.88839829\ldots$	$B(-1.15,-1.15) = -28.7414305\ldots$
⋮	⋮	⋮
87	[9.90623415, 9.90623418]	$[-3.46758381E+1, -3.46758376E+1]$
90	[9.94887452, 9.94887455]	$[-3.35679657E+1, -3.35679654E+1]$
101	[9.89577500, 9.89577505]	$[-3.2800630E+1, -3.2800628E+1]$
104	[9.92011383, 9.92011387]	$[-3.2057759E+1, -3.2057758E+1]$
116	[9.89154826, 9.89154835]	$[-3.155988E+1, -3.155986E+1]$
119	[9.90552580, 9.90552586]	$[-3.1050792E+1, -3.1050790E+1]$
132	[9.8897991, 9.8897993]	$[-3.071807E+1, -3.071806E+1]$
135	[9.89785968, 9.89785978]	$[-3.036422E+1, -3.036420E+1]$
149	[9.8890471, 9.8890474]	$[-3.013697E+1, -3.013695E+1]$
152	[9.8937091, 9.8937093]	$[-2.988867E+1, -2.988865E+1]$
167	[9.8887101, 9.8887106]	$[-2.973114E+1, -2.973111E+1]$
170	[9.8914122, 9.8914126]	$[-2.955578E+1, -2.955576E+1]$
186	[9.8885530, 9.8885537]	$[-2.94455E+1, -2.94454E+1]$
189	[9.8901217, 9.8901222]	$[-2.932109E+1, -2.932106E+1]$
206	[9.888477, 9.888479]	$[-2.92434E+1, -2.92432E+1]$
209	[9.8893889, 9.8893897]	$[-2.91549E+1, -2.91547E+1]$
227	[9.888439, 9.888441]	$[-2.90999E+1, -2.90996E+1]$
230	[9.888969, 9.888971]	$[-2.90367E+1, -2.90365E+1]$
249	[9.888419, 9.888423]	$[-2.8998E+1, -2.8997E+1]$
252	[9.888728, 9.888731]	$[-2.89526E+1, -2.89523E+1]$
272	[9.888408, 9.888413]	$[-2.8925E+1, -2.8924E+1]$
275	[9.888588, 9.888592]	$[-2.8893E+1, -2.8892E+1]$
296	[9.888401, 9.888409]	$[-2.8874E+1, -2.8871E+1]$
299	[9.888507, 9.888513]	$[-2.8850E+1, -2.8849E+1]$
321	[9.888394, 9.888410]	$[-2.884E+1, -2.883E+1]$
324	[9.888457, 9.888469]	$[-2.8820E+1, -2.8817E+1]$
347	[9.88838, 9.88842]	$[-2.882E+1, -2.880E+1]$
350	[9.88842, 9.88845]	$[-2.880E+1, -2.879E+1]$
374	[9.88836, 9.88844]	$[-2.881E+1, -2.877E+1]$
377	[9.88838, 9.88845]	$[-2.879E+1, -2.877E+1]$
402	[9.8882, 9.8886]	$[-2.89E+1, -2.87E+1]$
405	[9.887, 9.890]	$[-2.89E+1, -2.87E+1]$
⋮	⋮	⋮

Table 6

definitions of multivariate Padé approximants which can be found in the literature. An overview is given in [10]. In these earlier definitions the notion of "degree" was rigidly fixed (either square-like or triangular-like degree sets for both numerator and denominator) and hence no extra dimension of choice was introduced to deal

with the complexity of the multivariate problem. The ability to combine different of these approaches when using the general order multivariate Padé approximant defined by (1) is essential and it should be exploited fully. For didactical purposes we have built up our numerical case study gradually, displaying many non-meaningful multivariate Padé approximants, but it should be obvious that when interested in an approximation for the Beta function in $(-0.75, -0.75)$, we would only have computed the multivariate Padé approximants displayed in Table 6, in this way obtaining quite nice approximation results.

7. Special Case

The approach we have taken in the previous sections to define and construct multivariate Padé approximants is essentially based on rewriting the double series expansion

$$\sum_{(i,j)\in\mathbf{N}^2} c_{ij}x^i y^j \tag{15}$$

as the single sum

$$\sum_{r_I(i,j)=0}^{\infty} c_{ij}x^i y^j$$

In general, a numbering r_I of $\mathbf{N}^t$ places the points in $\mathbf{N}^t$ one after the other. By doing so, the dimension of the problem description is reduced in two ways. Firstly, the explicit determinant representation of the solution as well as the E- and *qdg*-algorithms for its computation depend on the numbering r_I in $\mathbf{N}^t$ and not on the number t of variables: the input is indexed by integer numbers $r_I(i_1,\ldots,i_t) \in \mathbf{N}$ and not by multi-indices $(i_1,\ldots,i_t) \in \mathbf{N}^t$. Secondly, the E- and *qdg*-algorithms are also applicable for univariate problems: the dimension of the output table and the dimension of the table of intermediate g-values are the same as when univariate input is used. Further simplifications of the algorithms to compute multivariate Padé approximants are only possible for special cases which we shall discuss now.

Another way to work with the bivariate power series (15) is the following

$$\sum_{(i,j)\in\mathbf{N}^2} c_{ij}x^i y^j = \sum_{\ell=0}^{\infty} \left(\sum_{i+j=\ell} c_{ij}x^i y^j \right)$$

This approach is taken in [8, p. 59–62] to construct homogeneous multivariate Padé approximants. These homogeneous multivariate Padé approximants are a special case of the general definition (1) where for chosen ν and μ in $\mathbf{N}$, substituting the degrees n and m in the univariate Padé approximant $[n/m]_{n+m}$, the numerator and

denominator degree sets N and D are given by

$$\begin{aligned} N &= \{(i,j) \in \mathbf{N}^2 \mid \nu\mu \leq i+j \leq \nu\mu+\nu\} \\ D &= \{(d,e) \in \mathbf{N}^2 \mid \nu\mu \leq d+e \leq \nu\mu+\mu\} \end{aligned} \tag{16}$$

while

$$\begin{aligned} I &= I_{(\nu,\mu)} \cup I_\Phi \\ I_{(\nu,\mu)} &= \{(i,j) \in \mathbf{N}^2 \mid \nu\mu \leq i+j \leq \nu\mu+\nu+\mu\} \\ I_\Phi &= \{(i,j) \in \mathbf{N}^2 \mid 0 \leq i+j < \nu\mu\} \\ \#I_{(\nu,\mu)} &= \#N + \#D - 1 \end{aligned}$$

The conditions in I_Φ are automatically satisfied by the choice of N and D and hence void. We shall denote these homogeneous multivariate Padé approximants by $[\nu/\mu]_{I(\nu,\mu)}$. Since they are a special case of the general order multivariate Padé approximants (1) the determinant representation (6) and the algorithms (8) and (10) remain valid for homogeneous Padé approximants. However, an advantage of homogeneous Padé approximants is that they preserve the properties and the nature of univariate Padé approximants even better than the general order definition (1). This is for instance reflected in a tremendous simplification of the algorithms for their computation. To see this, we introduce the notation

$$\begin{aligned} A_\ell(x,y) &= \sum_{i+j=\nu\mu+\ell} a_{ij}x^iy^j \qquad \ell = 0,\ldots,\nu \\ B_\ell(x,y) &= \sum_{i+j=\nu\mu+\ell} b_{ij}x^iy^j \qquad \ell = 0,\ldots,\mu \\ C_\ell(x,y) &= \sum_{i+j=\ell} c_{ij}x^iy^j \qquad \ell = 0,1,2\ldots \end{aligned}$$

and rewrite

$$\begin{aligned} p(x,y) &= \sum_{(i,j)\in N} a_{ij}x^iy^j = \sum_{\ell=0}^{\nu} A_\ell(x,y) \\ q(x,y) &= \sum_{(i,j)\in D} b_{ij}x^iy^j = \sum_{\ell=0}^{\mu} B_\ell(x,y) \end{aligned}$$

Then the conditions

$$(fq-p)(x,y) = \sum_{(i,j)\in\mathbf{N}^2\setminus I} d_{ij}x^iy^j = \sum_{i+j\geq\nu\mu+\nu+\mu+1} d_{ij}x^iy^j$$

can be reformulated as

$$\begin{cases} C_0(x,y)B_0(x,y) = A_0(x,y) \\ C_1(x,y)B_0(x,y) + C_0(x,y)B_1(x,y) = A_1(x,y) \\ \quad \vdots \\ C_\nu(x,y)B_0(x,y) + \ldots + C_{\nu-\mu}(x,y)B_\mu(x,y) = A_\nu(x,y) \end{cases}$$

$$\begin{cases} C_{\nu+1}(x,y)B_0(x,y) + \ldots + C_{\nu+1-\mu}(x,y)B_\mu(x,y) = 0 \\ \quad \vdots \\ C_{\nu+\mu}(x,y)B_0(x,y) + \ldots + C_\nu(x,y)B_\mu(x,y) = 0 \end{cases}$$

where $C_\ell(x,y) \equiv 0$ if $\ell < 0$. From this system of defining equations, the following determinant representation for multivariate homogeneous Padé approximants can easily be deduced [5]

$$\frac{p(x,y)}{q(x,y)} = \frac{\begin{vmatrix} \sum_{\ell=0}^{\nu} C_\ell(x,y) & \sum_{\ell=0}^{\nu-1} C_\ell(x,y) & \ldots & \sum_{\ell=0}^{\nu-\mu} C_\ell(x,y) \\ C_{\nu+1}(x,y) & C_\nu(x,y) & \ldots & C_{\nu+1-\mu}(x,y) \\ \vdots & & \ddots & \vdots \\ C_{\nu+\mu}(x,y) & \ldots & & C_\nu(x,y) \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \ldots & 1 \\ C_{\nu+1}(x,y) & C_\nu(x,y) & \ldots & C_{\nu+1-\mu}(x,y) \\ \vdots & & \ddots & \vdots \\ C_{\nu+\mu}(x,y) & \ldots & & C_\nu(x,y) \end{vmatrix}} \tag{17}$$

This is exactly the determinant representation for univariate Padé approximants if the univariate term $c_\ell x^\ell$ is substituted by

$$C_\ell(x,y) = \sum_{i+j=\ell} c_{ij} x^i y^j \qquad \ell = 0, 1, 2 \ldots$$

We remark that compared to the determinant representation (6), the size of the determinants in (17) has been reduced from $\#D = (3\mu + \mu^2)/2 + \nu\mu(\mu+1) + 1$ to $\mu + 1$. This is a significant simplification, especially if one computes the value of the homogeneous Padé approximant (for instance with LSS) as the first unknown

of the system

$$\begin{pmatrix} 1 & 1 & \dots & 1 \\ C_{\nu+1}(x,y) & C_{\nu}(x,y) & \dots & C_{\nu+1-\mu}(x,y) \\ \vdots & & \ddots & \vdots \\ C_{\nu+\mu}(x,y) & \dots & & C_{\nu}(x,y) \end{pmatrix}^T \begin{pmatrix} x_0 \\ \\ \vdots \\ x_\mu \end{pmatrix} = \begin{pmatrix} \sum_{\ell=0}^{\nu} C_\ell(x,y) \\ \sum_{\ell=0}^{\nu-1} C_\ell(x,y) \\ \vdots \\ \sum_{\ell=0}^{\nu-\mu} C_\ell(x,y) \end{pmatrix}$$

instead of as the first unknown of the system of equations (7).

By performing the same substitution of $c_\ell x^\ell$ by $C_\ell(x,y)$ in the starting values of the univariate ϵ-algorithm and the univariate qd-algorithm, these univariate algorithms also remain valid for the computation of multivariate homogeneous Padé approximants. More precisely, for the multivariate ϵ-algorithm the starting values and the continuation rules are given by

$$\begin{aligned} \epsilon_{-1}^{(k)} &= 0 \\ \epsilon_{0}^{(k)} &= \sum_{i+j=0}^{k} c_{ij}x^iy^j = \sum_{\ell=0}^{k} C_\ell(x,y) \qquad k=0,\dots,\nu+\mu \\ \epsilon_{\ell+1}^{(k)} &= \epsilon_{\ell-1}^{(k+1)} + \frac{1}{\epsilon_\ell^{(k+1)} - \epsilon_\ell^{(k)}} \end{aligned}$$

and $\epsilon_{2\mu}^{(\nu-\mu)} = [\nu/\mu]_{I(\nu,\mu)}$ [5].

What concerns the qd-algorithm, the univariate qd-algorithm is first rewritten in a form such that it can immediately be generalized. If the univariate Padé approximant $[\nu/\mu]_{\nu+\mu}$ is the $2\mu^{th}$ convergent of the continued fraction

$$\sum_{i=0}^{\nu-\mu} c_i x^i + \cfrac{c_{\nu-\mu+1}x^{\nu-\mu+1}}{1} + \cfrac{-q_1^{(\nu-\mu+1)}x}{1} + \cfrac{-e_1^{(\nu-\mu+1)}x}{1} + \dots$$

then we can also say that $[\nu/\mu]_{\nu+\mu}$ is the $2\mu^{th}$ convergent of the continued fraction

$$\sum_{i=0}^{\nu-\mu} c_i x^i + \cfrac{c_{\nu-\mu+1}x^{\nu-\mu+1}}{1} + \cfrac{-Q_1^{(\nu-\mu+1)}}{1} + \cfrac{-E_1^{(\nu-\mu+1)}}{1} + \dots \qquad (18)$$

Including the factor x in $Q_\ell^{(k)}$ and $E_\ell^{(k)}$ does not change the computation rules of

the qd-algorithm except for the starting values. More explicitly

$$\begin{aligned} E_0^{(k)} &= 0 \\ Q_1^{(k)} &= \frac{c_{k+1}x^{k+1}}{c_k x^k} \\ E_\ell^{(k)} &= E_{\ell-1}^{(k+1)} + Q_\ell^{(k+1)} - Q_\ell^{(k)} \\ Q_{\ell+1}^{(k)} &= Q_\ell^{(k+1)} \frac{E_\ell^{(k+1)}}{E_\ell^{(k)}} \end{aligned}$$

If we now perform the substitution of $c_\ell x^\ell$ by $C_\ell(x,y)$ in the starting values, namely

$$Q_1^{(k)} = \frac{C_{k+1}(x,y)}{C_k(x,y)} = \frac{\sum_{i+j=k+1} c_{ij}x^i y^j}{\sum_{i+j=k} c_{ij}x^i y^j}$$

then we have that the $2\mu^{th}$ convergent of (18) is the $[\nu/\mu]_{I(\nu,\mu)}$ multivariate homogeneous Padé approximant [7]. Again, note that this algorithm is much simpler than the qdg-algorithm (10), where the $[\nu/\mu]_{I(\nu,\mu)}$ homogeneous Padé approximant is computed as the $(2\cdot\#D)^{th}$ convergent, in other words the $((3\mu+\mu^2)+2\nu\mu(\mu+1)+2)^{th}$ convergent, of the continued fraction (9).

From the above it is clear that the restriction (16) on the numerator and denominator degree of multivariate homogeneous Padé approximants is compensated by the algorithmic simplicity with which they can be computed. Another important advantage they have over general order Padé approximants is that they have a unique irreducible form and as a consequence satisfy the consistency property [8, p. 65], meaning that if $f(x,y)$ is a rational function then, for suitably chosen homogeneous degrees in numerator and denominator, the homogeneous Padé approximant for $f(x,y)$ retrieves the function $f(x,y)$. The general order multivariate Padé approximants defined by (1) only satisfy the consistency property if the linear system of defining equations (3b) has maximal rank.

Let us now return to our numerical example. We have pointed out above, that if one is interested in approximating the function $f(x-1,y-1)$ in any point (u_i,v_j) where

$$(u_i,v_j) \in \{(x,y) : x > -2, y > -2, (x+1)(y+1) \neq 0\}$$

then one should look at symmetric Padé approximants with fixed denominator degree set D_3 given by (13). However, because of the restrictions (16) imposed on the numerator and denominator degree sets of homogeneous Padé approximants, the denominator degree set of a homogeneous Padé approximant can never be of the form (13). To compare the homogeneous with the general order multivariate Padé approximants, we compute $[\nu/\mu]_{I(\nu,\mu)}$ approximants with $\mu = 1$ or 2 and $\nu = 0,1,2,\ldots$ for the function $f(x-1,y-1)$ in $(-1.15,-1,15)$. The value of

ν \ μ	1	2
10	[−68.83305892, −6.883305890]	[−3.06182496, −3.06182493]
11	[−49.89056272, −4.989056268]	[−3.0791861, −3.0791860]
12	[−41.43546286, −4.143546281]	[−3.0127364, −3.0127362]
13	[−36.90202050, −3.690202043]	[−2.9532424, −2.9532422]
14	[−34.2004025, −34.2004023]	[−29.15540, −29.15539]
15	[−32.4816926, −32.4816923]	[−28.95002, −28.95000]
16	[−31.342539, −31.342538]	[−28.84588, −28.84585]
17	[−30.567672, −30.567670]	[−28.7943, −28.7941]
18	[−30.03173, −30.03172]	[−28.7685, −28.7683]
19	[−29.65693, −29.65692]	[−28.7556, −28.7553]
20	[−29.39291, −29.39289]	[−28.750, −28.748]
21	[−29.20598, −29.20596]	[−28.745, −28.743]
22	[−29.0731, −29.0730]	[−28.76, −28.75]
23	[−28.9795, −28.9793]	[−28.76, −28.75]
24	[−28.914, −28.913]	[−28.69, −28.65]
25	[−28.862, −28.861]	[−29.02, −29.00]
26	[−28.782, −28.780]	[−28.818, −28.816]
27	[−28.85, −28.84]	[−28.789, −28.786]
28	[−28.25, −28.23]	[−28.75, −28.74]
29	[−31.39, −31.37]	[−25.8, −25.7]
30	[−38.75, −38.70]	[−33.93, −33.90]

Table 7

the homogeneous Padé approximants in $(-1.15, -1.15)$ is computed by solving the linear system of equations (17) with LSS. The output is given in Table 7.

We recall that the denominator degree set of the $[\nu/\mu]_{I(\nu,\mu)}$ Padé approximant is of the form

$$D = \{(d,e) \mid \nu\mu \leq d+e \leq \nu\mu+\mu\} \qquad \#D = (3\mu+\mu^2)/2+\nu\mu(\mu+1)+1$$

Therefore, increasing the numerator degree ν of the homogeneous Padé approximant also increases the denominator degree set D. Hence a sequence of homogeneous Padé approximants $\{[\nu/\mu]_{I(\nu,\mu)}\}_{\nu\in\mathbf{N}}$ with fixed denominator degree μ does not correspond to a subsequence of any column in the table of general order multivariate Padé approximants. This immediately implies that Theorem 6 cannot be applied to any sequence of the form $\{[\nu/\mu]_{I(\nu,\mu)}\}_{\nu\in\mathbf{N}}$. Another type of de Montessus de Ballore theorem has been proved for homogeneous multivariate Padé approximants [9]. Moreover, a generalization of Theorem 5 on the convergence in measure of diagonal homogeneous Padé approximants is currently under investigation. That there is evidence for such convergence in measure is illustrated numerically in Table 8, which displays the value of diagonal homogeneous Padé approximants $[\nu/\nu]_{I(\nu,\nu)}$ in $(-0.75, -0.75)$.

ν	$B(-0.75,-0.75) = 9.88839829\ldots$
4	[8.3778971232, 8.3778971235]
5	[9.416025955, 9.416025961]
6	[9.90393140, 9.90393150]
7	[9.8862579, 9.8862582]
8	[9.888225, 9.888229]
9	[9.88839, 9.88841]

Table 8

We remark that because ν and μ play the same role for multivariate homogeneous Padé approximants as n and m for univariate Padé approximants, the notion of diagonal approximant is very natural for multivariate homogeneous Padé approximants. It suffices to let $\nu = \mu$. For general order multivariate Padé approximants the notion of diagonal approximant is not so clear because of the possibility to choose r_N different from r_D.

The results in Table 7 are comparable to those in Table 6 because, like the homogeneous Padé approximants in Table 7, the successive general order Padé approximants in Table 6, considered in pairs of two, enlarge their index set I with a full diagonal of index points. In order to make a comparison between Table 6 and Table 7, we should compare entries with the same informational usage, in other words entries which use the same amount of data. Clearly, the informational usage of the approximant $[N_k/D_\ell]_{I_{k+\ell}}$ is $\#I_{k+\ell} = k+\ell+1$. As is indicated in [6] and as can also be seen from the expressions $C_\ell(x,y)$ appearing in the determinant formula (17), the approximant $[\nu/\mu]_{I(\nu,\mu)}$ uses the coefficients c_{ij} with $0 \le i+j \le \nu+\mu$ and hence its informational usage is $(\nu+\mu+1)(\nu+\mu+2)/2$. Therefore, the entries

$$[N_k/D_\ell]_{I_{k+\ell}} \qquad k+\ell+1 = \frac{(s+1)(s+2)}{2} \qquad s = 0, 1, \ldots$$

in Table 6 and the entries

$$[\nu/\mu]_{I(\nu,\mu)} \qquad \nu+\mu = s \qquad s = 0, 1, \ldots$$

in Table 7 are comparable. For example, the general order Padé approximant $[N_{186}/D_3]_{I_{189}}$ and the homogeneous Padé approximants $[17/1]_{I(17,1)}$ and $[16/2]_{I(16,2)}$ are all constructed with the same amount of data. Identifying the midpoint of the interval output for each of these respective approximants with the approximant

itself, we find via (11b) that, as can be expected

$$\left| B(-1.15,-1.15) - \frac{1+(-2.15)(-2.15)[17/1]_{I(17,1)}}{(-1.15)(-1.15)} \right|$$

$$\leq \left| B(-1.15,-1.15) - \frac{1+(-2.15)(-2.15)[N_{186}/D_3]_{I_{189}}}{(-1.15)(-1.15)} \right|$$

$$\leq \left| B(-1.15,-1.15) \frac{1+(-2.15)(-2.15)[17/2]_{I(16,2)}}{(-1.15)(-1.15)} \right|$$

8. Conclusion

In this paper we have aimed at motivating the need for knowledge and reliability when dealing with multivariate approximation problems in general, and with multivariate Padé approximants in particular. That more and still better knowledge is needed in order to handle the complexity and the large number of choices when constructing multivariate Padé approximants has been illustrated through several numerical examples and is a source of current and future research.

We have emphasized the importance of constructing Padé approximants with a free choice for numerator and denominator degree sets. We have also discussed the importance of the numbering r_I with respect to the input data c_{ij}. Further research has to point out the role of the numbering r_I, also with respect to the application of the multivariate de Montessus de Ballore theorem. Numerical experiments [18] have indicated that there is clearly a link, with far reaching consequences, between the numbering r_I of the data and the polyradius of the polydisc $B(0; R_1, R_2)$ in theorem 6. However, up to now this link is not at all obvious.

Concerning the reliability, a research project is currently carried out at the University of Antwerp to construct a floating-point implementation with significance monitoring. The idea is to use the same amount of storage as interval arithmetic but to obtain more accuracy and hence sharper bounds by using information which is available on the stack of the processor but which is lost when the floating-point number is stored to memory.

Appendix A: Linear System Solver Pseudocode*

```
procedure solvelinsystem(dim: integer);
var R, A: matrix[1..dim,1..dim] of real;
    B: matrix[1..dim,1..dim] of interval;
    xt, b: vector[1..dim] of real;
```

* The declarations and the code can easily be adapted to handle interval input for A and b

```
    xk1, xk, z: vector[1..dim] of interval;
    k: integer;
begin
read(A); read(b);
R:= inverse(A);
xt:= R*b;
z:= ##(b-A*xt); {## implements the exact scalar product and}
z:= R*z;        {returns an interval enclosing the result}
B:= ##(makeidentmatrix(dim) - R*A);
xk1:= z;
k:= 0;
repeat
   xk:= xk1;
   xk1:= z + B*xk;
   k:= k+1;
until (xk1 < xk) or (k=10);
if (k < 10)
then writeln('verified inclusion', xt+xk1)
else writeln('inclusion failed')
end
```

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