

## The QD-Algorithm and Multivariate Padé-Approximants

Dedicated to Prof. Dr. P. Henrici on the occasion of his 60th birthday

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**Summary.** The quotient-difference (QD) algorithm can be used to construct univariate Padé-approximants [1]. In this paper we see that it can also be used to construct the multivariate Padé-approximants introduced in [3], just by reformulating the quotient-difference algorithm as in Sect. 1. The multivariate Padé-approximants and the multivariate QD-scheme are treated in the Sects. 2 and 3 respectively. Thus for this type of multivariate Padé-approximants a link with the theory of multivariate continued fractions is established.

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### 0. Introduction

It is well-known that the quotient-difference algorithm can be used to compute Padé-approximants for a univariate function [1]. They are obtained then as convergents of a continued fraction.

Several authors already have tried to generalize the concept of Padé-approximants to the multivariate case. We refer to [2, 6–9]. For all those generalizations there is no link with continued fractions. Other authors have introduced multivariate continued fractions without really obtaining Padé-approximants [11]. But if the multivariate Padé-approximants are defined, using a shift of the degrees of numerator and denominator [3], then one can construct multivariate continued fractions that provide those Padé-approximants and thus one can use the QD-algorithm to compute them. The shift of the degrees is also necessary to obtain a nontrivial denominator, as will be illustrated. For an extensive study of the properties of this type of Padé-approximants the interested reader is referred to [4].

In the last section the newly introduced multivariate QD-scheme will be used to calculate approximations for the poles and zeros of the two-variable beta-function.

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### 1. The Quotient-Difference Scheme

Our presentation of the QD-algorithm differs slightly from the usual one. In the one-dimensional case the two approaches are equivalent; however our approach can be generalized to the multivariate case.

Let us consider a univariate function

$$f(x) = \sum_{k=0}^{\infty} c_k x^k$$

analytic in the origin.

We call the series  $f$  normal if

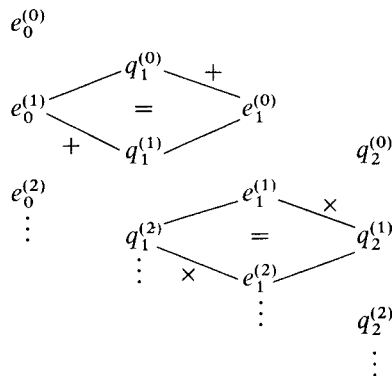
$$\begin{vmatrix} c_n x^n & c_{n+1} x^{n+1} & \dots & c_{n+k-1} x^{n+k-1} \\ c_{n+1} x^{n+1} & & & \\ \vdots & & & \\ c_{n+k-1} x^{n+k-1} & & & c_{n+2k-2} x^{n+2k-2} \end{vmatrix} \neq 0$$

for all  $n \geq 0$  and  $k \geq 1$ . This determinant is a monomial of degree  $k(n+k-1)$  in  $x$ . The condition of nontriviality is equivalent with the condition that the same determinant with  $x=1$  is nonzero.

For a normal series we can construct a table with double entry of numbers  $q_k^{(n)}$  and  $e_k^{(n)}$  defined as follows:

$$\begin{aligned} e_0^{(n)} &= 0 & n &= 0, 1, \dots, \\ q_1^{(n)} &= \frac{c_{n+1} x^{n+1}}{c_n x^n} & n &= 0, 1, \dots, \\ e_k^{(n)} &= q_k^{(n+1)} + e_{k-1}^{(n+1)} - q_k^{(n)} & n &= 0, 1, 2, \dots \quad k = 1, 2, \dots, \\ q_{k+1}^{(n)} &= q_k^{(n+1)} e_k^{(n+1)} / e_k^{(n)} & n &= 0, 1, 2, \dots \quad k = 1, 2, \dots \end{aligned}$$

These rules can easily be remembered by means of the following scheme (the superscript  $(n)$  indicates a diagonal while the subscript  $k$  indicates a column):



The QD-algorithm can now be used to construct Padé-approximants to the function  $f$ . For a normal series the Padé-table is likewise normal [1].

The  $(\ell, m)$  Padé-approximant (numerator of degree  $\ell$  and denominator of degree  $m$ ) for  $\ell \geq m$  is equal to the  $(2m)$ <sup>th</sup> convergent  $K_{2m}$  of the continued fraction

$$c_0 + c_1 x + \dots + c_{\ell-m} x^{\ell-m} + \cfrac{c_{\ell-m+1} x^{\ell-m+1}}{1} \cfrac{q_1^{(\ell-m+1)}}{1} \cfrac{e_1^{(\ell-m+1)}}{1} \cfrac{q_2^{(\ell-m+1)}}{1} \cfrac{e_2^{(\ell-m+1)}}{1} \dots$$

if  $K_0 = \sum_{k=0}^{\ell-m} c_k x^k$ , and the  $(2m+1)$ <sup>th</sup> convergent  $K_{2m+1}$  of the continued fraction

$$c_0 + c_1 x + \dots + c_{\ell-m-1} x^{\ell-m-1} + \cfrac{c_{\ell-m} x^{\ell-m}}{1} \cfrac{q_1^{(\ell-m)}}{1} \cfrac{e_1^{(\ell-m)}}{1} \cfrac{q_2^{(\ell-m)}}{1} \cfrac{e_2^{(\ell-m)}}{1} \dots$$

if  $K_0 = \sum_{k=0}^{\ell-m-1} c_k x^k$  [1].

The terms  $q_k^{(n)}$  and  $e_k^{(n)}$  each contain a factor  $x$  now because of the definition of  $q_1^{(n)}$ . We shall find this property also in the multivariate QD-scheme.

### 2. Multivariate Padé-Approximants

During the last ten years several ways have been tried to generalize the concept of Padé-approximant to multivariate functions. For most of the generalizations there is no link with continued fractions. The definition of the multivariate Padé-approximant which follows, enables one to construct multivariate continued fractions, the convergents of which provide the Padé-approximants.

Let

$$f(x_1, \dots, x_p) = \sum_{k_1, \dots, k_p=0}^{\infty} c_{k_1 \dots k_p} x_1^{k_1} \dots x_p^{k_p}.$$

If we introduce the notation

$$c_k(x) = \sum_{k_1 + \dots + k_p = k} c_{k_1 \dots k_p} x_1^{k_1} \dots x_p^{k_p}$$

we can also write for  $f(x_1, \dots, x_p)$ :

$$f(x) = \sum_{k=0}^{\infty} c_k(x)$$

where now  $x = (x_1, \dots, x_p)$  is a vector.

Now find

$$p_{[\ell, m]}(x) = \sum_{i=\ell m}^{\ell m + \ell} \sum_{i_1 + \dots + i_p = i} a_{i_1 \dots i_p} x_1^{i_1} \dots x_p^{i_p} = \sum_{i=\ell m}^{\ell m + \ell} a_i(x)$$

and

$$q_{[\ell, m]}(x) = \sum_{j=\ell m}^{\ell m+m} \sum_{j_1+\dots+j_p=j} b_{j_1\dots j_p} x_1^{j_1} \dots x_p^{j_p} = \sum_{j=\ell m}^{\ell m+m} b_j(x)$$

such that

$$(f \cdot q_{[\ell, m]} - p_{[\ell, m]})(x) = \sum_{k_1+\dots+k_p \geq \ell m + \ell + m + 1} d_{k_1\dots k_p} x_1^{k_1} \dots x_p^{k_p}. \tag{1}$$

If we denote by  $\partial_0$  the order of a power series, i.e. the degree of the first nonzero term (where a term  $x_1^{k_1} \dots x_p^{k_p}$  is said to be of degree  $k_1 + \dots + k_p$ ), then condition (1) can be reformulated as

$$\partial_0(f \cdot q_{[\ell, m]} - p_{[\ell, m]}) \geq \ell m + \ell + m + 1.$$

In the sequel of the text  $\partial$  will denote the degree of a polynomial.

The shift of the degrees of  $p_{[\ell, m]}(x)$  and  $q_{[\ell, m]}(x)$  by  $\ell m$  is necessary to obtain a nontrivial solution for the  $b_{j_1\dots j_p}$ . The following simple example will illustrate this.

Consider

$$f(x) = f(x_1, x_2) = 1 + x_1 + \sin(x_1 x_2) = 1 + x_1 + \sum_{k=0}^{\infty} (-1)^k \frac{(x_1 x_2)^{2k+1}}{(2k+1)!}.$$

Now take  $\ell = 1, m = 3$  and calculate

$$\begin{aligned} p(x_1, x_2) &= a_{00} + a_{10}x_1 + a_{01}x_2, \\ q(x_1, x_2) &= b_{00} + b_{10}x_1 + b_{01}x_2 + b_{20}x_1^2 + b_{11}x_1x_2 + b_{02}x_2^2 + b_{30}x_1^3 \\ &\quad + b_{21}x_1^2x_2 + b_{12}x_1x_2^2 + b_{03}x_2^3 \end{aligned}$$

such that

$$\partial_0(f \cdot q - p) \geq \ell + m + 1$$

i.e. without performing a shift in  $p, q$  and  $f \cdot q - p$ .

The only solution for  $p(x_1, x_2)$  and  $q(x_1, x_2)$  is

$$\begin{aligned} p(x_1, x_2) &\equiv 0, \\ q(x_1, x_2) &\equiv 0 \end{aligned}$$

which is useless.

A representation of  $p_{[\ell, m]}(x)$  and  $q_{[\ell, m]}(x)$  satisfying  $\partial_0(f \cdot q_{[\ell, m]} - p_{[\ell, m]}) \geq \ell m + \ell + m + 1$ , is

$$\begin{aligned} p_{[\ell, m]}(x) &= \begin{vmatrix} f_{\ell}(x) & f_{\ell-1}(x) & \dots & f_{\ell-m}(x) \\ c_{\ell+1}(x) & c_{\ell}(x) & \dots & c_{\ell-m+1}(x) \\ \vdots & & & \\ c_{\ell+m}(x) & & & c_{\ell}(x) \end{vmatrix}, \\ q_{[\ell, m]}(x) &= \begin{vmatrix} 1 & \dots & \dots & 1 \\ c_{\ell+1}(x) & c_{\ell}(x) & \dots & c_{\ell-m+1}(x) \\ \vdots & & & \\ c_{\ell+m}(x) & \dots & \dots & c_{\ell}(x) \end{vmatrix} \end{aligned}$$

where  $f_{\ell}(x) = \sum_{k=0}^{\ell} c_k(x)$ .

This is a direct generalization of the existing univariate formulas [10]. Observe that here the term

$$c_k(x) = \sum_{k_1 + \dots + k_p = k} c_{k_1 \dots k_p} x_1^{k_1} \dots x_p^{k_p}$$

takes the place of the coefficient  $c_k$ . This is precisely the difference between the usual definition of the QD-table and the one given in Sect. 1. More about this type of multivariate Padé-approximants can be found in [3].

### 3. The Multivariate QD-Scheme

We proceed exactly as in the univariate case.

We call the series  $f$  normal if

$$\begin{vmatrix} c_n(x) & c_{n+1}(x) & \dots & c_{n+k-1}(x) \\ c_{n+1}(x) & & & \vdots \\ \vdots & & & \vdots \\ c_{n+k-1}(x) & & & c_{n+2k-2}(x) \end{vmatrix} \neq 0$$

for all  $n \geq 0$  and  $k \geq 1$ , where now

$$c_k(x) = \sum_{k_1 + \dots + k_p = k} c_{k_1 \dots k_p} x_1^{k_1} \dots x_p^{k_p}.$$

For a normal series the irreducible form  $\frac{P_\Delta}{q_\Delta}(x)$  of  $\frac{P_{[\ell, m]}}{q_{[\ell, m]}}(x)$  satisfies

$$\begin{aligned} \partial_1 p_\Delta &= \partial p_\Delta - \partial_0 q_\Delta = \ell, \\ \partial_1 q_\Delta &= \partial q_\Delta - \partial_0 q_\Delta = m, \\ \partial_0(f \cdot q_\Delta - p_\Delta) &= \ell m + \ell + m + 1 \end{aligned}$$

and thus  $\frac{P_\Delta}{q_\Delta}(x)$  occurs only once in the Padé-table [4, pp. 61–62].

Define the table with double entry as follows:

$$\begin{aligned} e_0^{(n)} &= 0 & n &= 0, 1, \dots, \\ q_1^{(n)} &= \frac{c_{n+1}(x)}{c_n(x)} = \frac{\sum_{k_1 + \dots + k_p = n+1} c_{k_1 \dots k_p} x_1^{k_1} \dots x_p^{k_p}}{\sum_{k_1 + \dots + k_p = n} c_{k_1 \dots k_p} x_1^{k_1} \dots x_p^{k_p}} & n &= 0, 1, \dots, \\ e_k^{(n)} &= q_k^{(n+1)} + e_{k-1}^{(n+1)} - q_k^{(n)} & n &= 0, 1, 2, \dots \quad k = 1, 2, \dots, \\ q_{k+1}^{(n)} &= q_k^{(n+1)} e_k^{(n+1)} / e_k^{(n)} & n &= 0, 1, 2, \dots \quad k = 1, 2, \dots \end{aligned}$$

and construct the following continued fractions:  
(all the  $q_k^{(n)}$  and  $e_k^{(n)}$  exist because  $f$  is normal [5, pp. 610])



**Theorem 2.**  $\frac{p_{[\ell, m]}(x)}{q_{[\ell, m]}(x)}$  is the  $(2m)^{\text{th}}$  convergent of the continued fraction (2).

*Proof.* Let  $\frac{p_{[\ell-m+i, j]}(x)}{q_{[\ell-m+i, j]}(x)} = K_{i+j}$ ,  $i+j=0, 1, \dots$

It is possible to construct a continued fraction with convergents  $K_0, K_1, K_2, \dots$ .

This continued fraction has the form

$$K_0 + \cfrac{K_1 - K_0}{1} + \sum_{n=2}^{\infty} \cfrac{K_{n-1} - K_n}{\cfrac{K_{n-1} - K_{n-2}}{K_n - K_{n-2}}}$$

which can be written as

$$\sum_{k=0}^{\ell-m} c_k(x) + \cfrac{c_{\ell-m+1}(x)}{1} + \cfrac{K_1 - K_2}{K_2 - K_0} + \sum_{n=3}^{\infty} \cfrac{(K_{n-1} - K_n)(K_{n-2} - K_{n-3})}{(K_n - K_{n-2})(K_{n-1} - K_{n-3})}. \tag{4}$$

It is easy to verify that

$$\cfrac{K_1 - K_2}{K_2 - K_0} = q_1^{(\ell-m+1)} \quad \text{and} \quad \cfrac{(K_2 - K_3)(K_1 - K_0)}{(K_3 - K_1)(K_2 - K_0)} = e_1^{(\ell-m+1)}$$

using the representation of  $p_{[\ell-m, 0]}(x)$ ,  $q_{[\ell-m, 0]}(x)$ ,  $p_{[\ell-m+1, 0]}(x)$ ,  $q_{[\ell-m+1, 0]}(x)$ , ... given in the previous section.

Let us denote

$$\cfrac{(K_{n-1} - K_n)(K_{n-2} - K_{n-3})}{(K_n - K_{n-2})(K_{n-1} - K_{n-3})}$$

by  $A_1^{(\ell-m+1)}$  if  $n$  is even and by  $B_1^{(\ell-m+1)}$  if  $n$  is odd. We write also  $A_1^{(\ell-m+1)} = q_1^{(\ell-m+1)}$ . If we write down the continued fraction that is the even contraction of (4) (i.e. a continued fraction having as convergents the  $K_{2n}$  for  $n=0, 1, \dots$ ), we get

$$\sum_{k=0}^{\ell-m} c_k(x) + \cfrac{c_{\ell-m+1}(x)}{|1 - A_1^{(\ell-m+1)}|} - \cfrac{A_1^{(\ell-m+1)} B_1^{(\ell-m+1)}}{|1 - B_1^{(\ell-m+1)} - A_2^{(\ell-m+1)}|} - \dots \tag{5}$$

If we write down the continued fraction that is the odd contraction of (4) with  $\ell-m$  replaced by  $\ell-m-1$  (i.e. a continued fraction having as convergents the

$$\cfrac{p_{[\ell-m, 0]}(x)}{q_{[\ell-m, 0]}(x)}, \quad \cfrac{p_{[\ell-m+1, 1]}(x)}{q_{[\ell-m+1, 1]}(x)}, \quad \cfrac{p_{[\ell-m+2, 2]}(x)}{q_{[\ell-m+2, 2]}(x)}, \quad \dots$$

on the descending staircase (7)), we get

$$\sum_{k=0}^{\ell-m-1} c_k(x) + \cfrac{c_{\ell-m}(x) A_1^{(\ell-m)}}{|1 - A_1^{(\ell-m)} - B_1^{(\ell-m)}|} - \cfrac{B_1^{(\ell-m)} A_2^{(\ell-m)}}{|1 - A_2^{(\ell-m)} - B_2^{(\ell-m)}|} - \dots \tag{6}$$

Because (5) and (6) have the same convergents we have

$$A_k^{(\ell-m+1)} B_k^{(\ell-m+1)} = B_k^{(\ell-m)} A_{k+1}^{(\ell-m)} \quad k = 1, 2, \dots,$$

$$B_{k-1}^{(\ell-m+1)} + A_k^{(\ell-m+1)} = A_k^{(\ell-m)} + B_k^{(\ell-m)} \quad k = 1, 2, \dots$$

if we put  $B_0^{(\ell-m+1)} = 0$ .

So

$$A_k^{(\ell-m+1)} = q_k^{(\ell-m+1)}$$

$$B_k^{(\ell-m+1)} = e_k^{(\ell-m+1)} \quad k = 1, 2, \dots$$

This completes the proof.

Analogously we can formulate and prove the next theorem.

**Theorem 3.**  $\frac{P_{[\ell, m]}(x)}{q_{[\ell, m]}(x)}$  is the  $(2m + 1)^{\text{th}}$  convergent of the continued fraction (3).

This can easily be seen by writing down the continued fraction (4) with  $\ell - m$  replaced by  $\ell - m - 1$ ; the convergents of this continued fraction are the multivariate Padé-approximants on the following descending staircase:

$$\frac{P_{[\ell-m-1, 0]}(x)}{q_{[\ell-m-1, 0]}(x)}$$

$$\frac{P_{[\ell-m, 0]}(x)}{q_{[\ell-m, 0]}(x)} \quad \frac{P_{[\ell-m, 1]}(x)}{q_{[\ell-m, 1]}(x)} \tag{7}$$

$$\frac{P_{[\ell-m+1, 1]}(x)}{q_{[\ell-m+1, 1]}(x)} \quad \dots$$

$$\vdots$$

The following example both illustrates Theorems 2 and 3. Consider

$$f(x) = f(x_1, x_2) = \frac{x_1 e^{x_1} - x_2 e^{x_2}}{x_1 - x_2} = \sum_{i_1, i_2=0}^{\infty} \frac{x_1^{i_1} x_2^{i_2}}{(i_1 + i_2)!}$$

$$= 1 + x_1 + x_2 + \frac{1}{2}(x_1^2 + x_1 x_2 + x_2^2) + \dots$$

Take  $\ell = 2$  and  $m = 1$ . The Padé-approximant  $\frac{P_{[2, 1]}(x_1, x_2)}{q_{[2, 1]}}$  is given by

$$P_{[2, 1]}(x_1, x_2) = \left| \begin{array}{cc} 1 + x_1 + x_2 + \frac{1}{2}(x_1^2 + x_1 x_2 + x_2^2) & 1 + x_1 + x_2 \\ \frac{1}{6}(x_1^3 + x_1^2 x_2 + x_1 x_2^2 + x_2^3) & \frac{1}{2}(x_1^2 + x_1 x_2 + x_2^2) \end{array} \right|$$

$$= \frac{1}{2}(x_1^2 + x_1 x_2 + x_2^2) + \frac{1}{3}(x_1^3 + \frac{5}{2}(x_1^2 x_2 + x_1 x_2^2) + x_2^3)$$

$$+ \frac{1}{12}(x_1^4 + 2(x_1^3 x_2 + x_1 x_2^3) + 5x_1^2 x_2^2 + x_2^4)$$

$$q_{[2, 1]}(x_1, x_2) = \left| \begin{array}{cc} 1 & 1 \\ \frac{1}{6}(x_1^3 + x_1^2 x_2 + x_1 x_2^2 + x_2^3) & \frac{1}{2}(x_1^2 + x_1 x_2 + x_2^2) \end{array} \right|$$

$$= \frac{1}{2}(x_1^2 + x_1 x_2 + x_2^2) - \frac{1}{6}(x_1^3 + x_1^2 x_2 + x_1 x_2^2 + x_2^3).$$



According to Theorem 2, this is also the second convergent of the continued fraction (2), i.e.

$$1 + x_1 + x_2 + \cfrac{\cfrac{\frac{1}{2}(x_1^2 + x_1 x_2 + x_2^2)}{1}}{1} - \cfrac{\cfrac{\cfrac{(x_1^3 + x_1^2 x_2 + x_1 x_2^2 + x_2^3)}{3(x_1^2 + x_1 x_2 + x_2^2)}}{1}}{1}.$$

According to Theorem 3 it is also the third convergent of the continued fraction (3), i.e.

$$1 + \cfrac{x_1 + x_2}{1} - \cfrac{\cfrac{\cfrac{(x_1^2 + x_1 x_2 + x_2^2)}{2(x_1 + x_2)}}{1}}{1} - \cfrac{\cfrac{\cfrac{\cfrac{-(x_1^4 + 2x_1^3 x_2 + 5x_1^2 x_2^2 + 2x_1 x_2^3 + x_2^4)}{6(x_1^2 + x_1 x_2 + x_2^2)(x_1 + x_2)}}{1}}{1}}{1}.$$

In both cases the QD-scheme is started with

$$q_1^{(n)} = \sum_{i_1+i_2=n+1} \frac{x_1^{i_1} x_2^{i_2}}{(i_1+i_2)!} \bigg/ \sum_{i_1+i_2=n} \frac{x_1^{i_1} x_2^{i_2}}{(i_1+i_2)!}.$$

### 4. Numerical Example

The beta function is defined by

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

where  $\Gamma$  is the gamma function.

Singularities occur for  $x = -n$  and  $y = -n$  ( $n=0, 1, 2, \dots$ ) and zeros for  $y = -x - n$  ( $n=0, 1, 2, \dots$ ). We write

$$B(x, y) = \frac{A(x-1, y-1)}{xy}$$

with

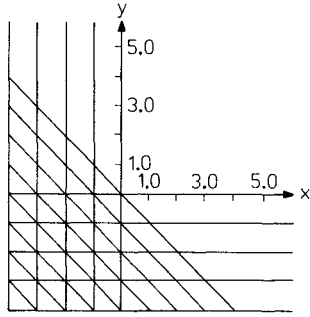
$$A(u, v) = 1 + uvf(u, v).$$

We will calculate the Padé-approximant  $p_{[\ell, m]}(u, v)/q_{[\ell, m]}(u, v)$  for  $f(u, v)$  by means of the multivariate QD-algorithm and compute

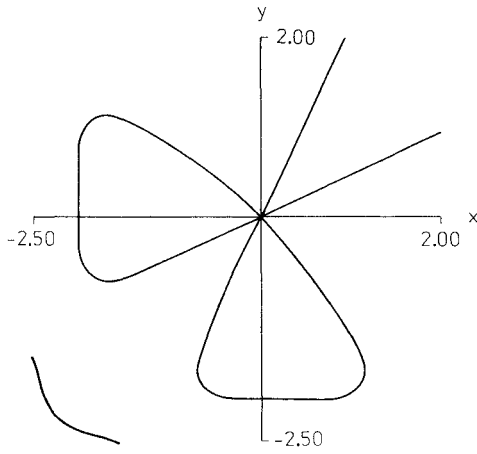
$$\frac{q_{[\ell, m]}(x-1, y-1) + (x-1)(y-1)p_{[\ell, m]}(x-1, y-1)}{xyq_{[\ell, m]}(x-1, y-1)} \tag{8}$$

as an approximation for  $B(x, y)$ .

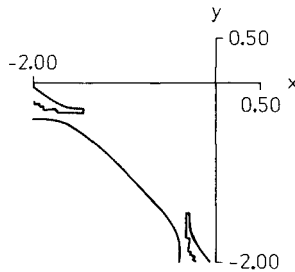
The trajectories of the poles and zeros of the beta function are shown in Fig. 1, while the poles of (8) for  $\ell=7$  and  $m=1$  and the zeros of (8) for  $\ell=2$  and  $m=2$  can respectively be found in Fig. 2 and Fig. 3.



**Fig. 1**



**Fig. 2**



**Fig. 3**

In both cases we remark that the vertical, horizontal and diagonal lines are nicely simulated, and that the drawings are symmetric because the symmetry of  $B(x, y)$  is preserved by the multivariate Padé-approximants [4].

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