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GENERAL ORDER MULTIVARIATE RATIONAL HERMITE INTERPOLANTS

ANNIE CUYT

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ABSTRACT

In the past two decades, several attempts were made to introduce multivariate Padé approximants and multivariate rational interpolants. We refer to [CHISc, GRAVa, HUGH, KARL, LUTTb, CUYTf, MURP, SIEM, CUYTj, CUYTk, KUCH, SKOR]. Each author used his or her own approach and no unifying theory existed except for the multivariate Padé approximants defined in [CUYTf]. In this work we present a definition of multivariate rational interpolants which was for the first time introduced in [CUYTi] and which fills a number of gaps in the results obtained up to now.

First of all the definition is a very general one in that sense that a lot of previously given multivariate Padé approximants are rediscovered as special cases, including the one given in [CUYTf]. The well-known univariate results in the theory of Padé approximation and rational Hermite interpolation are also found again.

Secondly the definition allows several equivalent approaches: one can set up a linear system of defining equations for the unknown numerator and denominator coefficients, one can start a recursive computation scheme to compute the value of the multivariate rational interpolant, one can write down a continued fraction and obtain the interpolant as a convergent.

This much more coherent theory of multivariate rational Hermite interpolation has a number of practical applications as well.

Some multidimensional convergence accelerators, introduced in the past, result from the use of these interpolants and hence profit from the new computational techniques. Some new convergence accelerators are born which improve the existing methods.

For the solution of systems of nonlinear equations a whole variety of nonlinear iterative procedures seems to be possible, by the fact that the iteration can be adapted to the available information for each of the nonlinear equations. By this we mean the possibility to evaluate or differentiate the equations easily. As is to be expected these nonlinear iterative procedures are to be preferred in the neighbourhood of singularities.

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1. STATE OF THE ART.

In the field of rational approximation and interpolation, many generalizations exist. We list a number of tools that have been created in the past years. They all make use of rational functions, but the approximation property they satisfy, is different. We shall also distinguish between the univariate and the multivariate case and indicate which new type of approximant is introduced here.

Let the univariate complex-valued function f be given by its series expansion around x_0

$$f(x) = \sum_{i=0}^{\infty} c_i (x - x_0)^i$$

or by some function values f_i in distinct complex points x_i ($i = 0, 1, 2, \ldots$).

For n and m chosen we construct polynomials

$$p(x) = \sum_{i=0}^{n} a_i x^i$$

and

$$q(x) = \sum_{i=0}^{m} b_i x^i$$

such that [CUYTl, pp. 129–155]

$$(fq - p)(x_i) = 0 \qquad i = 0, \ldots, n + m \tag{I.1.1}$$

It is clear that problem (I.1.1) always has a nontrivial solution for $p(x)$ and $q(x)$ since it is a homogeneous system of $n+m+1$ linear equations in $n+m+2$ unknowns a_i and b_i. Hence at least one unknown can be chosen freely. This problem is called the **rational interpolation problem** for f of order (n, m).

Suppose that in the sequence of interpolation points several subsequent points coincide. Let x_i occur $r_i + 1$ times in a row ($i = 0, 1, 2, \ldots$). Then problem (I.1.1) is reformulated as follows. Let n and m be chosen such that

$$n + m + 1 = \sum_{i=0}^{k} (r_i + 1)$$

Find polynomials $p(x)$ and $q(x)$ such that [WUYT]

$$(fq - p)^{(j)}(x_i) = 0 \qquad j = 0, \ldots, r_i \qquad i = 0, \ldots, k \tag{I.1.2}$$

This is called the **rational Hermite interpolation problem** for f of order (n, m).

The limiting case is when all the interpolation points coincide with one single point x_0. The conditions for the polynomials $p(x)$ and $q(x)$ then amount to [CUYTl, pp. 63–95]

$$(fq - p)(x_0) = \sum_{i=n+m+1}^{\infty} d_i (x - x_0)^i \tag{I.1.3}$$

Problem (I.1.3) is called the **Padé approximation problem** for f of order (n, m). Note that the linear system resulting from (I.1.3) uses the Taylor series expansion of f. This is because having several data in one single point is interpreted as knowing higher derivatives of that function in the point considered.

In [CLAEb] the rational Hermite interpolation problem is reformulated as a **Newton-Padé approximation problem.** In a formal manner we can construct with the data f_i the Newton interpolating series

$$f(x) = \sum_{i=0}^{\infty} f[x_0, \ldots, x_i] B_i(x)$$

where

$$B_i(x) = \prod_{j=0}^{i-1} (x - x_j) \qquad B_0(x) = 1$$

and $f[x_0, \ldots, x_i]$ is a divided difference with possible coalescence of points. We redefine

$$p(x) = \sum_{i=0}^{n} a_i B_i(x)$$

and

$$q(x) = \sum_{i=0}^{m} b_i B_i(x)$$

and compute the coefficients a_i and b_i such that

$$(fq - p)(x) = \sum_{i=n+m+1}^{\infty} d_i B_i(x) \qquad (I.1.4)$$

It is easy to see that the problems (I.1.2) and (I.1.4) are equivalent.

For each of the four problems considered it is always true that if p_1 and q_1 satisfy any of the conditions (I.1.1-I.1.4) and if p_2 and q_2 satisfy the same condition, then the rational functions constructed with these polynomials are equivalent, meaning that

$$p_1 q_2 = p_2 q_1$$

In this way the irreducible form of a solution of any of the four problems is unique and hence we can define it to be the **(n,m) rational interpolant** for f if we are dealing with problem (I.1.1), the **(n,m) rational Hermite interpolant** or the **(n,m) Newton-Padé approximant** if we're dealing with the problems (I.1.2) or (I.1.4) and the **(n,m) Padé approximant** for f if we are dealing with problem (I.1.3). In each of the four cases we shall denote the irreducible form by $r_{n,m}$.

Up to now we have considered linear conditions. The rational function $r_{n,m}$ can be considered as the root of the linear equation

$$q r_{n,m} - p = 0$$

where p and q are determined by any of the interpolation or approximation conditions (I.1.1-I.1.4). Instead of such linear equations one can also consider algebraic equations

$$\sum_{i=0}^{k} r^i_{m_0,\ldots,m_k} p_i = 0$$

where the polynomials p_i of degree m_i are determined by

$$\sum_{i=0}^{k} f^i(x)p_i(x) = \sum_{i=\ell}^{\infty} d_i B_i(x) \qquad \ell = m_0 + \ldots + m_k + k + 1 \qquad (I.1.5)$$

An extensive study of this type of problems is made in [DELL] and [LÜBB]. When $k = 2$ and all the interpolation points coincide, the rational function r_{m_0,m_1,m_2} is called the **quadratic approximant** for f [SHAF] since it is the root of the quadratic equation

$$r^2_{m_0,m_1,m_2} p_2 + r_{m_0,m_1,m_2} p_1 + p_0 = 0$$

with

$$f^2(x)p_2(x) + f(x)p_1(x) + p_0(x) = \sum_{i=m_0+m_1+m_2+3}^{\infty} d_i x^i$$

Up to now we have also only used the basis functions x^i or $B_i(x)$ to span the polynomial ring that contains the elements $p(x)$ and $q(x)$. One could also use linear combinations

$$p(x) = \sum_{i=0}^{n} a_i g_i(x)$$

and

$$q(x) = \sum_{i=0}^{m} b_i g_i(x)$$

of basis functions $g_i(x)$, which we call generalized polynomials, and study the **generalized interpolation or approximation problem**

$$(fq - p)^{(j)}(x_i) = 0 \qquad j = 0, \ldots, r_i \qquad i = 0, \ldots, k \qquad (I.1.6)$$

Examples of such interpolation problems can be found in [MÜHL] and [LOI].

Padé approximants are in fact a special case of so-called Padé-type approximants [BREZe]. In this type of problem a rational function $r_{n,m}$

with numerator and denominator respectively of degree at most n and m is computed such that

$$(fq - p)(x) = \sum_{i=n+1}^{\infty} d_i (x - x_0)^i \qquad (I.1.7)$$

Condition (I.1.7) supplies us with a linear system of $n+1$ equations in $n+m+1$ unknowns. The remaining $m+1$ free parameters are used to insert some extra information about f if it is available, for instance some knowledge about singularities of f.

So far for the univariate one-dimensional case. Some of the above notions have been generalized to the multivariate case, some to the multidimensional case.
The problem is multidimensional when we are working with a k-tuple of univariate functions.
The problem is multivariate when a complex-valued function depends on k variables.
Multidimensional Padé approximants can be found in [DEBR], multidimensional rational interpolants in [GRAVb] and [WYNN].
Of multivariate Padé approximants several definitions exist. In [CUYTc] their advantages and drawbacks are discussed. Here we shall prove that some of them result as the limiting case of the multivariate rational Hermite interpolants we are going to introduce. In the past years an attempt has also been made to introduce multivariate quadratic approximants [CHISa, CHISb] and multivariate Pade-type approximants [BREZd] but the number of papers on the subject is very limited.

Our main aim is not to introduce another new concept but to establish a unifying theory that admits to see the wood for the trees again. That's why we have chosen the following reasoning.

It is well-known that univariate Padé approximants, which are a special case of univariate rational interpolants by letting all the interpolation points coincide, can be obtained in several equivalent ways: one can write down the system of linear equations that must be satisfied by the numerator and denominator coefficients, one can start a recursive computation scheme, one can consider convergents of corresponding continued fractions. Each of these three defining techniques is generalized by different authors to the multivariate case. However, the equivalence between the defining techniques is then lost [CUYTc] by the way in which the generalization was formulated. Let us study this matter in more detail.

When the technique of the defining equations [CHISc, HUGH, KARL, LEVIa, LUTTb] or the continued fraction approach [MURP, SIEM] is used to define multivariate Padé approximants, then the set of equations or the form of the continued fraction can be chosen so that many of the univariate properties carry over to the multivariate case. In fact you can force your approximant to satisfy a certain property by adding the right equations to your system or the right terms to your continued fraction. But it is not possible to give a linear system and a continued fraction expansion that generate the same rational approximant. Depending on what sort of approximant you want, you have to make your choice. On the other hand, if the quotient of determinants which can be computed recursively by means of the epsilon-algorithm, is preserved in the generalization [CUYTf, CUYTg], then it is possible to establish a link between different approaches [CUYTc]. For such multivariate Padé approximants based on a recursive scheme, one can give an equivalent linear system of defining equations and a corresponding continued fraction representation.

In this text we shall see that recursive schemes will again play an important role.
When we treat some special cases of the newly introduced multivariate rational Hermite interpolants, we shall prove that multivariate Padé approximants defined by means of a linear system of equations for their numerator and denominator coefficients, can be computed recursively by means of a generalization of the epsilon-algorithm [CUYTe]. Remember that the epsilon-algorithm is commonly used for the recursive computation of univariate Padé approximants.
We shall also see that multivariate Padé approximants that result from a defining system of linear equations can after all be obtained as the successive convergents of a continued fraction. We note that the computed continued fraction has a different form than the ones used up to now in multivariate interpolation and approximation theory: it is not branched.
Both these results are due to the fact that our definition of multivariate rational Hermite interpolants enables a very univariate-like determinant

representation which is of vital importance for the preservation of recursive epsilon-like algorithms. It is to be expected that these results create a whole lot of new algorithmic possibilities.

As a result of all this the equivalence of the three main defining techniques for univariate Padé approximants is re-established in the multivariate theory. While the reader makes his or her way through the next sections he or she will notice that this unification is not limited to the case of multivariate Padé approximants but that it is only a side result of the equivalence of the three main defining techniques in this new theory of multivariate rational Hermite interpolants.

2. MULTIVARIATE INTERPOLATION PROBLEMS.

For the sake of simplicity we restrict ourselves in the sequel of part I to the case of two variables. The generalization to the case of more than two variables will appear to be straightforward and only notationally more difficult. Let us first describe the conditions which have to be fulfilled by the multivariate data set before the interpolants can be constructed. Since we allow coalescence of interpolation points, we shall also point out how to deal with such a situation.

Consider for instance the following picture in $\mathbb{N}^2$ of the data set (x_i, y_j), where a circle indicates that in addition to $f_{ij} = f(x_i, y_j)$ also $\partial f/\partial x$ is given and a square indicates that also $\partial f/\partial x$, $\partial f/\partial y$ and $\partial^2 f/\partial y^2$ are provided.

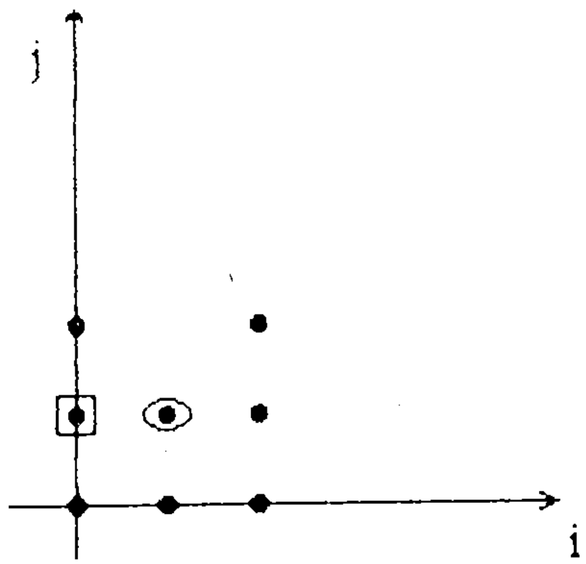

Figure I.2.1

This situation can be considered as the limit situation of a data set with non-coalescent interpolation points where we let $x_3 \to x_0$, $x_4 \to x_1$, $y_3 \to y_1$ and $y_4 \to y_1$.

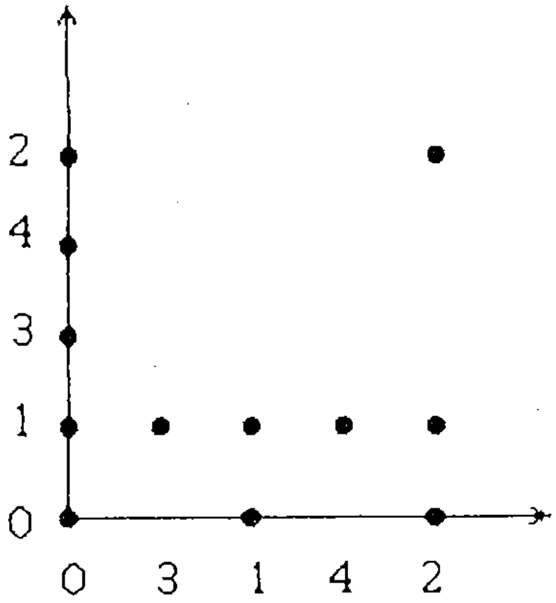

Figure I.2.2

If we want to interpolate these (x_i, y_j, f_{ij}) by means of the technique described in the following chapters, then the data f_{ij} and the numbering of the x_i and y_j have to be such that

(I.2.1a) x_0 is that x-coordinate for which the number of y-coordinates at which data are given is maximal, x_1 is the one of the leftover points for which the same is true, and so on

(I.2.1b) y_0 is that y-coordinate for which the number of x-coordinates at which data are given is maximal, y_1 is the one of the leftover points for which the same is true, and so on

(I.2.1c) the data set has the inclusion property, meaning that when a point belongs to the data set then the rectangular subset of points emanating from the origin with the given point as its furthermost corner also lies in the data set.

Note that (I.2.1a) and (I.2.1b) do not necessarily imply (I.2.1c). This is easily understood if one considers the data set $\{(x_0, y_0), (x_1, y_1), (x_2, y_2)\}$. We shall comment on the importance of condition (I.2.1c) in section 3. For the picture above this is clearly not the case. So we try to renumber the interpolation points such that these three conditions are satisfied. Let us introduce a new numbering (x'_i, y'_j) with

$$x'_0 = x_0 \quad x'_1 = x_2 \quad x'_2 = x_1 \quad x'_3 = x_4 \quad x'_4 = x_3$$

and

$$y'_0 = y_1 \quad y'_1 = y_0 \quad y'_2 = y_2 \quad y'_3 = y_4 \quad y'_4 = y_3$$

We then get the following picture in $\mathbb{N}^2$ of the data set.

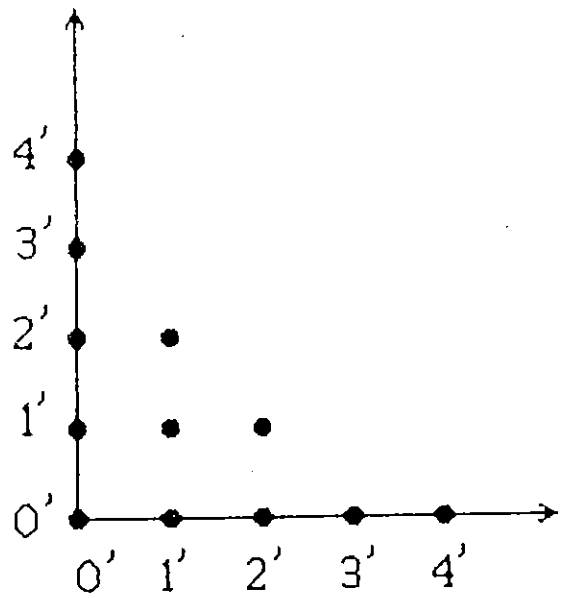

Figure I.2.3

The interpolation problems that can be reduced to this situation are of course not the most general ones but they already represent quite a number of situations that can be dealt with. In the sequel of the text we assume that the given data set is already structured such that the conditions (I.2.1) are fulfilled. This will enable us to adopt the notation (x_i, y_j) again instead of (x'_i, y'_j).

Let the complex function values f_{ij} be given in the complex points (x_i, y_j) with $(i,j) \in I \subseteq \mathbb{N}^2$, where I satisfies the inclusion property, meaning that when (i,j) belongs to I then (k,ℓ) belongs to I for $k \leq i$ and $\ell \leq j$. We know from the pictures above that a data set with coalescent interpolation points can be replaced by an intermediate data set where only function values are given. For a bivariate function $f(x,y)$ we define the following divided differences

$$f[x_0][y_0] = f(x_0, y_0)$$
$$f[x_0][y_0,\dots,y_k] = \frac{f[x_0][y_1,\dots,y_k] - f[x_0][y_0,\dots,y_{k-1}]}{y_k - y_0}$$
$$f[x_0,\dots,x_k][y_0] = \frac{f[x_1,\dots,x_k][y_0] - f[x_0,\dots,x_{k-1}][y_0]}{x_k - x_0}$$

$$f[x_0,\dots,x_k][y_0,\dots,y_\ell] = \frac{f[x_0,\dots,x_k][y_1,\dots,y_\ell] - f[x_0,\dots,x_k][y_0,\dots,y_{\ell-1}]}{y_\ell - y_0} \qquad (I.2.2a)$$

or equivalently

$$f[x_0,\dots,x_k][y_0,\dots,y_\ell] = \frac{f[x_1,\dots,x_k][y_0,\dots,y_\ell] - f[x_0,\dots,x_{k-1}][y_0,\dots,y_\ell]}{x_k - x_0} \qquad (I.2.2b)$$

One can easily prove that (I.2.2a) and (I.2.2b) give the same result.

LEMMA I.2.1. *The divided difference* $f[x_0,\dots,x_k][y_0,\dots,y_\ell]$ *is independent of the order of the points* $x_0,\dots,x_k$ *and* $y_0,\dots,y_\ell$.

PROOF: The proof is only a modification of the proof for univariate divided differences. ■

When certain interpolation points coincide, we must bear in mind the following remarks. Let r_i be a positive integer indicating that $r_i + 1$ of the x-coordinates in I coincide with x_i and let s_j indicate that $s_j + 1$ of the y-coordinates in I coincide with y_j . These coalescent x- and y-coordinates are not necessarily consecutive. To indicate which x- or

y-coordinates respectively coincide with x_i or y_j we can introduce the following notation. Let

$$i(0), \ldots, i(r_i)$$

denote the indices of the x-coordinates coinciding with x_i, and analogously let

$$j(0), \ldots, j(s_j)$$

denote the indices of the y-coordinates coinciding with y_j. For the calculation of the divided differences we then need the starting values

$$f[x_{i(0)}, \ldots, x_{i(k)}][y_j] = \frac{1}{k!} \frac{\partial^k f}{\partial x^k} |_{(x_i, y_j)} \qquad 0 \leq k \leq r_i$$

$$f[x_i][y_{j(0)}, \ldots, y_{j(\ell)}] = \frac{1}{\ell!} \frac{\partial^\ell f}{\partial y^\ell} |_{(x_i, y_j)} \qquad 0 \leq \ell \leq s_j$$

$$f[x_{i(0)}, \ldots, x_{i(k)}][y_{j(0)}, \ldots, y_{j(\ell)}] = \frac{1}{k!} \frac{1}{\ell!} \frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell} |_{(x_i, y_j)}$$
$$0 \leq k \leq r_i \qquad 0 \leq \ell \leq s_j$$

For the polynomials in two variables we consider the following set of basis functions:

$$B_{ij}(x, y) = \prod_{k=1}^{i} (x - x_{k-1}) \prod_{\ell=1}^{j} (y - y_{\ell-1})$$

This basis function is a bivariate polynomial of degree $i + j$. With $c_{0i,0j} = f[x_0, \ldots, x_i][y_0, \ldots, y_j]$ we can now write in a purely formal manner [BERE]

$$f(x, y) = \sum_{(i,j) \in \mathbb{N}^2} c_{0i,0j} B_{ij}(x, y) \qquad (I.2.3)$$

Hence we have constructed with the data a bivariate Newton interpolating series and we can start approximating it using bivariate rational functions. The next chapter will generalize condition (I.1.4.) and its solution to the bivariate case.

The following lemmas about products of basis functions $B_{ij}(x, y)$ and about bivariate divided differences of products of functions will play an important role in the sequel of the text.

LEMMA I.2.2. *For $k+\ell \geq i+j$ the product $B_{ij}(x,y)B_{k\ell}(x,y)$ is given by*

$$B_{ij}(x,y)B_{k\ell}(x,y) = \sum_{\mu=0}^{i}\sum_{\nu=0}^{j} \lambda_{\mu\nu} B_{k+\mu,\ell+\nu}(x,y)$$

PROOF: We write $B_{ij}(x,y) = B_{i0}(x,y)B_{0j}(x,y)$. Since $B_{i0}(x,y)$ is a polynomial in x of degree i we can write

$$B_{i0}(x,y) = \sum_{\mu=0}^{i} \alpha_\mu \left(\prod_{\gamma=k}^{k+\mu-1} (x - x_\gamma) \right)$$

and

$$B_{0j}(x,y) = \sum_{\nu=0}^{j} \beta_\nu \left(\prod_{\gamma=\ell}^{\ell+\nu-1} (y - y_\gamma) \right)$$

with the convention that an empty product is equal to 1. Consequently

$$\begin{aligned} B_{ij}(x,y)B_{k\ell}(x,y) &= [B_{k\ell}(x,y)B_{i0}(x,y)]B_{0j}(x,y) \\ &= \left[\sum_{\mu=0}^{i} \alpha_\mu B_{k+\mu,\ell}(x,y) \right] B_{0j}(x,y) \\ &= \sum_{\nu=0}^{j}\sum_{\mu=0}^{i} \alpha_\mu \beta_\nu B_{k+\mu,\ell+\nu}(x,y) \end{aligned}$$

which gives the desired formula if we put $\lambda_{\mu\nu} = \alpha_\mu \beta_\nu$. ■

A figure in $\mathbb{N}^2$ will clarify the meaning of this lemma. If we multiply $B_{ij}(x,y)$ by $B_{k\ell}(x,y)$ and $k+\ell \geq i+j$ then the only occuring $B_{\mu\nu}(x,y)$ in the product are those with (μ,ν) lying in the shaded rectangle.

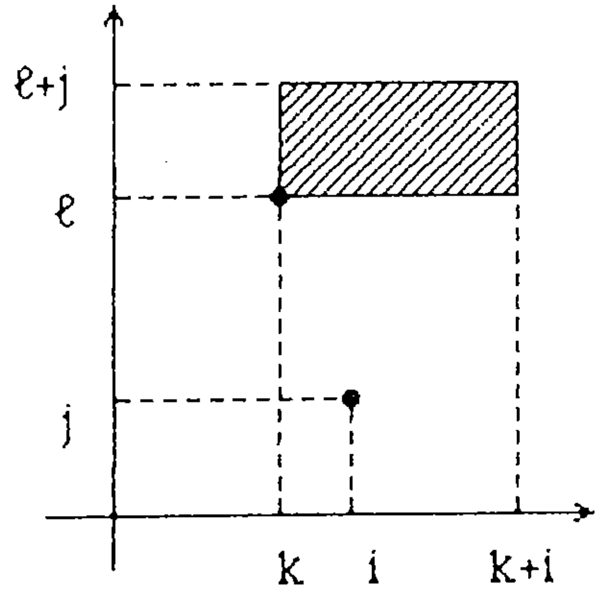

Figure I.2.4

LEMMA I.2.3.

$$(fq)[x_0,\ldots,x_i][y_0,\ldots,y_j] = \sum_{\mu=0}^{i}\sum_{\nu=0}^{j} f[x_0,\ldots,x_\mu][y_0,\ldots,y_\nu]\; q[x_\mu,\ldots,x_i][y_\nu,\ldots,y_j]$$

PROOF: The proof is by induction and analogous to the proof of the univariate case. ∎

3. Determinant representation of general order multivariate rational Hermite interpolants.

The definition of multivariate Newton-Padé approximants which we shall give is a very general one. It includes the univariate definition and a lot of the definitions for multivariate Padé approximants as a special case. With any finite subset D of $\mathbb{N}^2$ we associate a polynomial

$$\sum_{(i,j)\in D} b_{ij}B_{ij}(x,y)$$

Given the double Newton series

$$f(x,y) = \sum_{(i,j)\in \mathbb{N}^2} c_{0i,0j}B_{ij}(x,y)$$

with $c_{0i,0j} = f[x_0,\ldots,x_i][y_0,\ldots,y_j]$, we choose three subsets N, D and I of $\mathbb{N}^2$ and construct an $[N/D]_I$ Newton-Padé approximant to $f(x,y)$ as follows:

$$p(x,y) = \sum_{(i,j)\in N} a_{ij}B_{ij}(x,y) \qquad (N \text{ from “numerator”}) \tag{I.3.1a}$$

$$q(x,y) = \sum_{(i,j)\in D} b_{ij}B_{ij}(x,y) \qquad (D \text{ from “denominator”}) \tag{I.3.1b}$$

$$(fq-p)(x,y) = \sum_{(i,j)\in \mathbb{N}^2\setminus I} d_{ij}B_{ij}(x,y) \qquad (I \text{ from “interpolation conditions”}) \tag{I.3.1c}$$

In analogy with the univariate case, we select N, D and I such that
  D has $m+1$ elements, numbered $(d_0,e_0),\ldots,(d_m,e_m)$
  $N \subset I$
  I satisfies the rectangle rule:
    if $(i,j)\in I$ then $(k,\ell)\in I$ for $k\le i$ and $\ell \le j$

$I \backslash N$ has at least m elements.
Clearly the coefficients d_{ij} in

$$(fq-p)(x,y) = \sum_{(i,j)\in \mathbb{N}^2} d_{ij} B_{ij}(x,y)$$

are

$$d_{ij} = (fq-p)[x_0,\ldots,x_i][y_0,\ldots,y_j]$$

So the conditions (I.3.1c) are equivalent with

$$(fq-p)[x_0,\ldots,x_i][y_0,\ldots,y_j] = 0 \qquad (i,j)\in I \qquad (I.3.2)$$

Because $N \subset I$, the system of equations (I.3.2) can be divided into a nonhomogeneous and a homogeneous part:

$$(fq)[x_0,\ldots,x_i][y_0,\ldots,y_j] = p[x_0,\ldots,x_i][y_0,\ldots,y_j] \qquad (i,j)\in N \qquad (I.3.3a)$$

$$(fq)[x_0,\ldots,x_i][y_0,\ldots,y_j] = 0 \qquad (i,j)\in I\backslash N \qquad (I.3.3b)$$

Let's take a look at the conditions (I.3.3b). Suppose that I is such that exactly m of the homogeneous equations (I.3.3b) are linearly independent. We number the respective m elements in $I\backslash N$ with $(h_1,k_1),\ldots,(h_m,k_m)$ and define the set

$$H = \{(h_1,k_1),\ldots,(h_m,k_m)\} \subseteq I\backslash N \qquad (H \text{ from "homogeneous equations"})$$

By means of lemma I.2.3 we have

$$\begin{aligned}(fq)[x_0,\ldots,x_i][y_0,\ldots,y_j] &= (qf)[x_0,\ldots,x_i][y_0,\ldots,y_j] \\ &= \sum_{\mu=0}^{i}\sum_{\nu=0}^{j} q[x_0,\ldots,x_\mu][y_0,\ldots,y_\nu] f[x_\mu,\ldots,x_i][y_\nu,\ldots,y_j]\end{aligned}$$

Since the only nontrivial $q[x_0,\ldots,x_\mu][y_0,\ldots,y_\nu]$ are the ones with (μ,ν) in D we can write

$$(fq)[x_0,\ldots,x_i][y_0,\ldots,y_j] = \sum_{(\mu,\nu)\in D} b_{\mu\nu} f[x_\mu,\ldots,x_i][y_\nu,\ldots,y_j]$$

Remember that $f[x_\mu,\dots,x_i][y_\nu,\dots,y_j]=0$ if $\mu>i$ or $\nu>j$. So the homogeneous system of m equations in $m+1$ unknowns looks like

$$\begin{pmatrix} c_{d_0h_1,e_0k_1} & \cdots & c_{d_mh_1,e_mk_1} \\ \vdots & & \vdots \\ c_{d_0h_m,e_0k_m} & \cdots & c_{d_mh_m,e_mk_m} \end{pmatrix} \begin{pmatrix} b_{d_0,e_0} \\ \vdots \\ b_{d_m,e_m} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \qquad (I.3.4)$$

because

$$D=\{(d_0,e_0),\dots,(d_m,e_m)\}$$

As we suppose the rank of the coefficient matrix to be maximal, a solution $q(x,y)$ is given by

$$q(x,y)=\begin{vmatrix} B_{d_0e_0}(x,y) & \dots & B_{d_me_m}(x,y) \\ c_{d_0h_1,e_0k_1} & \cdots & c_{d_mh_1,e_mk_1} \\ \vdots & & \vdots \\ c_{d_0h_m,e_0k_m} & \cdots & c_{d_mh_m,e_mk_m} \end{vmatrix} \qquad (I.3.5a)$$

By the conditions (I.3.3a) and lemma I.2.3 we find

$$\begin{aligned} p(x,y) &= \sum_{(i,j)\in N} a_{ij}B_{ij}(x,y) \\ &= \sum_{(i,j)\in N} p[x_0,\dots,x_i][y_0,\dots,y_j]B_{ij}(x,y) \\ &= \sum_{(i,j)\in N} (qf)[x_0,\dots,x_i][y_0,\dots,y_j]B_{ij}(x,y) \\ &= \sum_{(\mu,\nu)\in D} b_{\mu\nu}\left(\sum_{(i,j)\in N} c_{\mu i,\nu j}B_{ij}(x,y)\right) \end{aligned}$$

Consequently a determinant representation for $p(x,y)$ is given by

$$p(x,y)=\begin{vmatrix} \sum_{(i,j)\in N} c_{d_0i,e_0j}B_{ij}(x,y) & \dots & \sum_{(i,j)\in N} c_{d_mi,e_mj}B_{ij}(x,y) \\ c_{d_0h_1,e_0k_1} & \cdots & c_{d_mh_1,e_mk_1} \\ \vdots & & \vdots \\ c_{d_0h_m,e_0k_m} & \cdots & c_{d_mh_m,e_mk_m} \end{vmatrix} \qquad (I.3.5b)$$

If for all k, $\ell \geq 0$ we have $q(x_k, y_\ell) \neq 0$ then $\frac{1}{q}(x, y)$ can be written as

$$\frac{1}{q}(x,y) = \sum_{(i,j)\in \mathbb{N}^2} e_{ij} B_{ij}(x,y)$$

with $e_{ij} = \frac{1}{q}[x_0, \ldots, x_i][y_0, \ldots, y_j]$. Hence by the use of lemma I.2.2 and since I satisfies the inclusion property

$$(f - \frac{p}{q})(x,y) = \left[\frac{1}{q}(fq - p)\right](x,y) = \sum_{(i,j)\in \mathbb{N}^2 \setminus I} \tilde{d}_{ij} B_{ij}(x,y)$$

If I does not satisfy the inclusion property, as in the next figure,

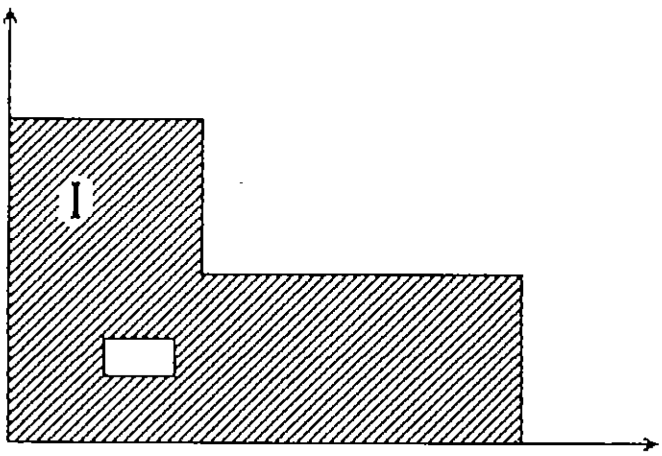

Figure I.3.1

then

$$(fq - p)(x,y) = \sum_{(i,j)\in \mathbb{N}^2 \setminus I} d_{ij} B_{ij}(x,y)$$

does not imply

$$(f - \frac{p}{q})(x,y) = \sum_{(i,j)\in \mathbb{N}^2 \setminus I} \tilde{d}_{ij} B_{ij}(x,y)$$

since in that case $f - p/q$ also contains the terms that result from multiplying the "hole" by $\frac{1}{q}(x, y)$.

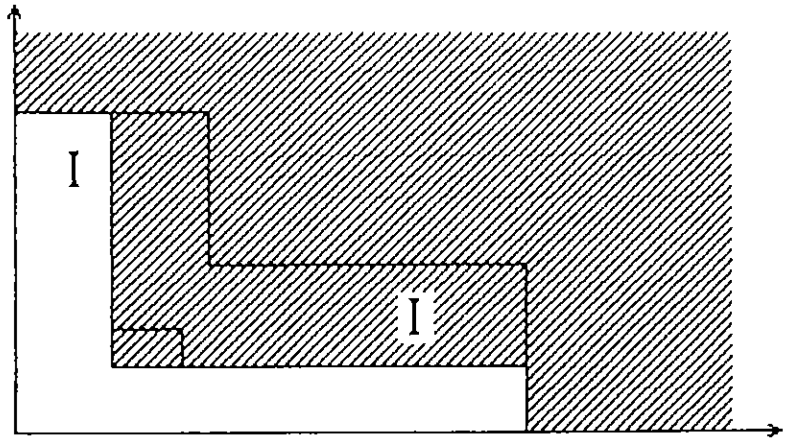

Figure I.3.2

The following theorem describes exactly which interpolation conditions are satisfied by p/q.

THEOREM I.3.1. *If $q(x_k, y_\ell) \neq 0$ for (k, ℓ) in I and if coinciding* x- *and* y-*coordinates have consecutive numbers*

$$x_k = x_{k+1} = \ldots = x_{k+r_k}$$
$$y_\ell = y_{\ell+1} = \ldots = y_{\ell+s_\ell}$$

then

$$\frac{\partial^{\mu+\nu} f}{\partial x^\mu \partial y^\nu}(x_k, y_\ell) = \frac{\partial^{\mu+\nu}(\frac{p}{q})}{\partial x^\mu \partial y^\nu}(x_k, y_\ell)$$

for

$$(\mu, \nu) \in E = \{(\mu, \nu) \mid 0 \leq \mu \leq r_k, 0 \leq \nu \leq s_\ell\} \cap \{(\mu, \nu) \mid (k+\mu, \ell+\nu) \in I\}$$

If $r_k = 0 = s_\ell$ this reduces to

$$f(x_k, y_\ell) = (\frac{p}{q})(x_k, y_\ell)$$

PROOF: Given r_k and s_ℓ for fixed (x_k, y_ℓ), consider the following situation for the interpolation points, with respect to I and define

$$\mu_I = \max\{\mu \mid x_{k+\mu} = x_k \text{and} (k+\mu, \ell) \in I\}$$
$$\nu_I = \max\{\nu \mid y_{\ell+\nu} = y_\ell \text{and} (k, \ell+\nu) \in I\}$$
$$\mu_C = \max\{\mu \mid \forall \nu, 0 \le \nu \le \nu_I : (k+\mu, \ell+\nu) \in I\}$$
$$\nu_C = \max\{\nu \mid \forall \mu, 0 \le \mu \le \mu_I : (k+\mu, \ell+\nu) \in I\}$$

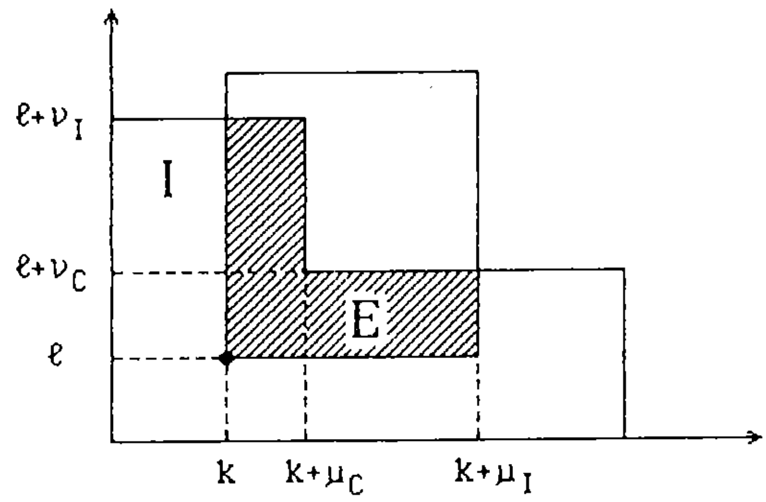

Figure I.3.3

Using these definitions we rewrite E as

$$E = E_1 \cup E_2$$

with

$$E_1 = \{(\mu, \nu) \mid 0 \le \mu \le \mu_I, 0 \le \nu \le \nu_C\}$$
$$E_2 = \{(\mu, \nu) \mid 0 \le \mu \le \mu_C, 0 \le \nu \le \nu_I\}$$

Because $q(x_k, y_\ell) \neq 0$ for (k, ℓ) in I we have

$$(f - \frac{p}{q})(x, y) = \sum_{(i,j) \in \mathbb{N}^2 \setminus I} \tilde{d}_{ij} B_{ij}(x, y)$$

To check the interpolation conditions we write

$$\begin{aligned}\frac{\partial^{\mu+\nu} B_{ij}}{\partial x^\mu \partial y^\nu} &= \frac{\partial^{\mu+\nu}(B_{i0}B_{0j})}{\partial x^\mu \partial y^\nu} \\ &= \frac{\partial^\mu}{\partial x^\mu}\left(\frac{\partial^\nu}{\partial y^\nu} B_{i0}B_{0j}\right) \\ &= \frac{\partial^\mu B_{i0}}{\partial x^\mu}\frac{\partial^\nu B_{0j}}{\partial y^\nu}\end{aligned}$$

If we cover $\mathbb{N}^2 \backslash I$ with three regions

$$\begin{aligned}A &= \{(i,j) \in \mathbb{N}^2 \backslash I \mid i > \mu_I\} \\ B &= \{(i,j) \in \mathbb{N}^2 \backslash I \mid j > \nu_I\} \\ C &= \{(i,j) \in \mathbb{N}^2 \backslash I \mid \mu_C < i \leq \mu_I, \nu_C < j \leq \nu_I\}\end{aligned}$$

then for (i,j) in A and (μ,ν) in E

$$\frac{\partial^\mu B_{i0}}{\partial x^\mu} \Big|_{(x_k,y_\ell)} = 0$$

because $B_{i0}(x,y)$ contains a factor $(x-x_k)^{\mu_I+1}$, and for (i,j) in B and (μ,ν) in E

$$\frac{\partial^\nu B_{0j}}{\partial y^\nu} \Big|_{(x_k,y_\ell)} = 0$$

Analogously for (i,j) in C and (μ,ν) in E_2

$$\frac{\partial^\mu B_{i0}}{\partial x^\mu} \Big|_{(x_k,y_\ell)} = 0$$

and for (i,j) in C and (μ,ν) in E_1

$$\frac{\partial^\nu B_{0j}}{\partial y^\nu} \Big|_{(x_k,y_\ell)} = 0$$

Finally for (μ,ν) in E and (k,ℓ) in I

$$\frac{\partial^{\mu+\nu}(f - \frac{p}{q})}{\partial x^\mu \partial y^\nu} \Big|_{(x_k,y_\ell)} = 0$$

The most general situation for the interpolation points with respect to I is slightly more complicated but completely analogous to the one given in figure I.3.3. We illustrate this remark by means of figure I.3.4.

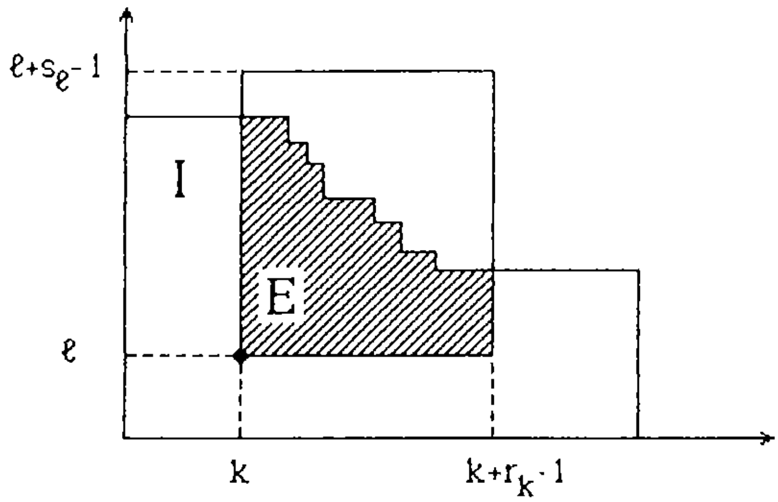

Figure I.3.4

The proof in this case is performed in the same way as above. ■

From the determinant representations (I.3.5a) and (I.3.5b) we can obtain the determinant representation given in [CLAEc] for univariate Newton-Padé approximants. Consider the Newton interpolating series for $f(x,0)$ and choose

$$D = \{(d,0) \mid 0 \le d \le m\}$$
$$N = \{(i,0) \mid 0 \le i \le n\}$$
$$I = \{(i,0) \mid 0 \le i \le n+m\}$$

If the points $\{(i,0) \mid n+1 \le i \le n+m\}$ supply linearly independent equations, then the determinant representations for $p(x,0)$ and $q(x,0)$

are

$$q(x,0) = \begin{vmatrix} 1 & (x-x_0) & \dots & \prod_{k=0}^{m-1}(x-x_k) \\ c_{0\;n+1,0\;0} & c_{1\;n+1,0\;0} & \dots & c_{m\;n+1,0\;0} \\ \vdots & \vdots & & \vdots \\ c_{0\;n+m,0\;0} & c_{1\;n+m,0\;0} & \dots & c_{n\;n+m,0\;0} \end{vmatrix}$$

$$p(x,0) = \begin{vmatrix} \sum_{i=0}^{n} c_{0i,00} \prod_{k=0}^{i-1}(x-x_k) & \dots & \sum_{i=0}^{n} c_{mi,00} \prod_{k=0}^{i-1}(x-x_k) \\ c_{0\;n+1,0\;0} & \dots & c_{m\;n+1,0\;0} \\ \vdots & & \vdots \\ c_{0\;n+m,0\;0} & \dots & c_{m\;n+m,0\;0} \end{vmatrix}$$

Let us now illustrate this multivariate setting by calculating a Newton-Padé approximant for

$$f(x,y) = 1 + \frac{x}{0.1-y} + \sin(xy)$$

with

$$x_i = i\sqrt{\pi} \qquad i = 0,1,2,\dots$$
$$y_j = (j-1)\sqrt{\pi} \qquad j = 0,1,2,\dots$$

The Newton interpolating series looks like

$$f(x,y) = 1 + \frac{1}{0.1+\sqrt{\pi}}x + \frac{10}{0.1+\sqrt{\pi}}x(y+\sqrt{\pi}) + \frac{10}{0.01-\pi}x(y+\sqrt{\pi})y + \sum_{i+j\geq 4} c_{0_i,0_j} B_{ij}(x,y)$$

Choose

$$D = \{(0,0),(1,0),(0,1)\}$$
$$N = \{(0,0),(1,0),(0,1),(1,1)\}$$
$$I = \{(2,0),(2,1),(0,2),(1,2)\}$$

Writing down the system of equations (I.3.3b), it is easy to check that

$$H = \{(2,1),(1,2)\}$$

The determinant formulas for $p(x,y)$ and $q(x,y)$ yield

$$q(x,y) = \begin{vmatrix} 1 & x & y+\sqrt{\pi} \\ c_{02,01} & c_{12,11} & c_{02,11} \\ c_{01,02} & c_{11,02} & c_{01,12} \end{vmatrix}$$
$$= \frac{100}{0.01-\pi}\left(1 - \frac{1}{0.1+\sqrt{\pi}}(y+\sqrt{\pi})\right)$$

$$p(x,y) = \begin{vmatrix} N_{00}(x,y) & N_{10}(x,y) & N_{01}(x,y) \\ c_{02,01} & c_{12,11} & c_{02,11} \\ c_{01,02} & c_{11,02} & c_{01,12} \end{vmatrix}$$

with

$$N_{00}(x,y) = \sum_{i=0}^{1}\sum_{j=0}^{1} c_{0i,0j}B_{ij}(x,y)$$
$$= 1 + \frac{x}{0.1+\sqrt{\pi}} + \frac{10}{0.1+\sqrt{\pi}}x(y+\sqrt{\pi})$$

$$N_{10}(x,y) = \sum_{i=0}^{1}\sum_{j=0}^{1} c_{1i,0j}B_{ij}(x,y)$$
$$= \frac{0.1+2\sqrt{\pi}}{0.1+\sqrt{\pi}}x + \frac{\sqrt{\pi}}{0.1(0.1+\sqrt{\pi})}x(y+\sqrt{\pi})$$

$$N_{01}(x,y) = \sum_{i=0}^{1}\sum_{j=0}^{1} c_{0i,1j}B_{ij}(x,y)$$
$$= (y+\sqrt{\pi}) + 10x(y+\sqrt{\pi})$$

Finally we obtain

$$[N/D]_I(x,y) = \frac{p}{q}(x,y) = \frac{0.1+\sqrt{\pi}+x-(y+\sqrt{\pi})}{0.1+\sqrt{\pi}-(y+\sqrt{\pi})}$$
$$= \frac{0.1+x-y}{0.1-y}$$

4. Recursive computation.

In order to construct rational interpolants that satisfy the interpolation conditions described by the set $I \subseteq \mathbb{N}^2$, we have chosen two finite index sets N, a subset of I, and D, a subset of $\mathbb{N}^2$, and we have put

$$p(x,y) = \sum_{(i,j)\in N} a_{ij} B_{ij}(x,y)$$

$$q(x,y) = \sum_{(i,j)\in D} b_{ij} B_{ij}(x,y)$$

$$(fq-p)(x,y) = \sum_{(i,j)\in \mathbb{N}^2\setminus I} c_{ij} B_{ij}(x,y)$$

Let us now introduce a numbering $r(i,j)$ of the points in $\mathbb{N}^2$ based on the enumeration

$$(0,0),\ \underbrace{(1,0),(0,1),}_{\text{first diagonal}}\ \underbrace{(2,0),(1,1),(0,2),}_{\text{second diagonal}}\underbrace{(3,0),(2,1),(1,2),(0,3)}_{\text{third diagonal}},\ldots$$

so that

$$r(i,j) = \frac{(i+j)(i+j+1)}{2} + j - i$$

If we denote

$$\#N = n+1$$

then we can write

$$N = \bigcup_{\ell=0}^{n} N_\ell$$

with

$$\emptyset = N_{-1} \subset N_0 \subset N_1 \subset \ldots \subset N_{n-1} \subset N_n = N$$

$$\#N_\ell = \ell + 1$$

$$N_\ell \setminus N_{\ell-1} = \{(i_\ell, j_\ell)\} \qquad \ell = 0,1,\ldots,n$$

$$r(i_\ell, j_\ell) > r(i_k, j_k) \qquad \ell > k$$

In other words, for each $\ell = 0, ..., n$ we add to $N_{\ell-1}$ the point (i_ℓ, j_ℓ) which is the next in line in $N \cap I\!N^2$ according to the enumeration given above.

Denote

$$\#D = m + 1$$

and proceed in the same way. Hence

$$D = \bigcup_{\ell=0}^{m} D_\ell$$

with

$$D_{-1} = \emptyset \qquad D_\ell \setminus D_{\ell-1} = \{(d_\ell, e_\ell)\} \qquad \ell = 0, ..., m$$

We have assumed that the interpolation set I is such that exactly m of the homogeneous equations are linearly independent. It is obvious that this condition guarantees the existence of a nontrivial solution because the number of unknowns in the homogeneous system is one more than its rank. We have also grouped the respective m elements in $I \setminus N$ that supply the linearly independent equations in the set H. If we number them according to the enumeration given above, we get

$$H = \bigcup_{\ell=1}^{m} H_\ell \subseteq I \setminus N$$

with

$$H_0 = \emptyset \qquad H_\ell \setminus H_{\ell-1} = \{(h_\ell, k_\ell)\} \qquad \ell = 1, ..., m$$

To obtain a recursive algorithm, the determinant formulas (I.3.5) for the polynomials $p(x, y)$ and $q(x, y)$ are rewritten as follows. Multiply the $(\ell + 1)^{th}$ row in $p(x, y)$ and $q(x, y)$ by $B_{h_\ell k_\ell}(x, y)$ $(\ell = 1, ..., m)$, and then divide the $(\ell + 1)^{th}$ column by $B_{d_\ell e_\ell}(x, y)$ $(\ell = 0, ..., m)$. This results in

$$p(x,y) =$$

$$\begin{vmatrix} \sum_{(i,j)\in N} c_{d_0 i, e_0 j} B_{d_0 i, e_0 j}(x,y) & \dots & \sum_{(i,j)\in N} c_{d_m i, e_m j} B_{d_m i, e_m j}(x,y) \\ c_{d_0 h_1, e_0 k_1} B_{d_0 h_1, e_0 k_1}(x,y) & \dots & c_{d_m h_1, e_m k_1} B_{d_m h_1, e_m k_1}(x,y) \\ \vdots & & \vdots \\ c_{d_0 h_m, e_0 k_m} B_{d_0 h_m, e_0 k_m}(x,y) & \dots & c_{d_m h_m, e_m k_m} B_{d_m h_m, e_m k_m}(x,y) \end{vmatrix}$$

$$q(x,y) =$$

$$\begin{vmatrix} 1 & \dots & 1 \\ c_{d_0 h_1, e_0 k_1} B_{d_0 h_1, e_0 k_1}(x,y) & \dots & c_{d_m h_1, e_m k_1} B_{d_m h_1, e_m k_1}(x,y) \\ \vdots & & \vdots \\ c_{d_0 h_m, e_0 k_m} B_{d_0 h_m, e_0 k_m}(x,y) & \dots & c_{d_m h_m, e_m k_m} B_{d_m h_m, e_m k_m}(x,y) \end{vmatrix}$$

where for $k \le i$ and $\ell \le j$

$$B_{ki,\ell j}(x,y) = \frac{B_{ij}(x,y)}{B_{k\ell}(x,y)} = (x - x_k)\dots(x - x_{i-1})(y - y_\ell)\dots(y - y_{j-1})$$

and for $k > i$ or $\ell > j$

$$c_{ki,\ell j} = 0$$

We can now easily construct $(m+1)$ series of which the successive partial sums can be found in the columns of $p(x,y)$. Take

$$t_0(0) = c_{d_0 i_0, e_0 j_0} B_{d_0 i_0, e_0 j_0}(x,y)$$

$$\Delta t_0(\ell - 1) = t_0(\ell) - t_0(\ell - 1) = c_{d_0 i_\ell, e_0 j_\ell} B_{d_0 i_\ell, e_0 j_\ell}(x,y) \qquad \ell = 1, ..., n$$

Then

$$t_0(n) = \sum_{(i,j)\in N} c_{d_0 i, e_0 j} B_{d_0 i, e_0 j}(x,y)$$

The next terms are given by

$$\begin{aligned} \Delta t_0(n + \ell - 1) &= t_0(n + \ell) - t_0(n + \ell - 1) \\ &= c_{d_0 h_\ell, e_0 k_\ell} B_{d_0 h_\ell, e_0 k_\ell}(x,y) \qquad \ell = 1, \dots, m \end{aligned}$$

Note that $\Delta t_0(\ell-1) = 0$ as long as $i_\ell < d_0$ or $j_\ell < e_0$ and $\Delta t_0(n+\ell-1) = 0$ as long as $h_\ell < d_0$ or $k_\ell < e_0$. In this way we obtain the first column of $p(x,y)$.

We can proceed in the same way for the other columns. Define for $r = 1, ..., m$

$$t_r(0) = c_{d_r i_0, e_r j_0} B_{d_r i_0, e_r j_0}(x,y)$$

$$\Delta t_r(\ell-1) = t_r(\ell) - t_r(\ell-1) = c_{d_r i_\ell, e_r j_\ell} B_{d_r i_\ell, e_r j_\ell}(x,y) \qquad \ell = 1, \dots, n$$

$$\begin{aligned} \Delta t_r(n+\ell-1) &= t_r(n+\ell) - t_r(n+\ell-1) \\ &= c_{d_r h_\ell, e_r k_\ell} B_{d_r h_\ell, e_r k_\ell}(x,y) \qquad \ell = 1, \dots, m \end{aligned}$$

Hence

$$t_r(n) = \sum_{(i,j)\in N} c_{d_r i, e_r j} B_{d_r i, e_r j}(x,y)$$

and the $(r+1)^{th}$ column of $p(x,y)$ is obtained. Again $\Delta t_r(\ell-1) = 0$ for $i_\ell < d_r$ or $j_\ell < e_r$ and $\Delta t_r(n+\ell-1) = 0$ for $h_\ell < d_r$ or $k_\ell < e_r$. Consequently

$$p(x,y) = \begin{vmatrix} t_0(n) & \dots & t_m(n) \\ \Delta\, t_0(n) & \dots & \Delta\, t_m(n) \\ \vdots & & \vdots \\ \Delta\, t_0(n+m-1) & \dots & \Delta\, t_m(n+m-1) \end{vmatrix} \qquad (I.4.1a)$$

$$q(x,y) = \begin{vmatrix} 1 & \dots & 1 \\ \Delta\, t_0(n) & \dots & \Delta\, t_m(n) \\ \vdots & & \vdots \\ \Delta\, t_0(n+m-1) & \dots & \Delta\, t_m(n+m-1) \end{vmatrix} \qquad (I.4.1b)$$

This quotient of determinants can easily be computed using the E-algorithm [BREZb]:

$$E_0^{(\ell)} = t_0(\ell) \qquad \ell = 0, \ldots, n+m$$

$$g_{0,r}^{(\ell)} = t_r(\ell) - t_{r-1}(\ell) \qquad r = 1, \ldots, m \qquad \ell = 0, \ldots, n+m$$

$$E_r^{(\ell)} = \frac{E_{r-1}^{(\ell)} g_{r-1,r}^{(\ell+1)} - E_{r-1}^{(\ell+1)} g_{r-1,r}^{(\ell)}}{g_{r-1,r}^{(\ell+1)} - g_{r-1,r}^{(\ell)}} \qquad \ell = 0, 1, \ldots, n \qquad r = 1, 2, \ldots, m \tag{I.4.2a}$$

$$g_{r,s}^{(\ell)} = \frac{g_{r-1,s}^{(\ell)} g_{r-1,r}^{(\ell+1)} - g_{r-1,s}^{(\ell+1)} g_{r-1,r}^{(\ell)}}{g_{r-1,r}^{(\ell+1)} - g_{r-1,r}^{(\ell)}} \qquad s = r+1, r+2, \ldots \tag{I.4.2b}$$

The values $E_r^{(\ell)}$ and $g_{r,s}^{(\ell)}$ are stored as in table I.4.1 and table I.4.2.

$$\begin{array}{lllll}
E_0^{(0)} & & & & \\
 & E_1^{(0)} & & & \\
 & & \ddots & & \\
E_0^{(1)} & & & & \\
 & E_1^{(1)} & & E_m^{(0)} & \\
E_0^{(2)} & \vdots & & \vdots & \ddots \\
\vdots & & & & E_{n+m}^{(0)} \\
 & & & E_m^{(n)} & \\
 & E_1^{(n+m-1)} & & & \\
E_0^{(n+m)} & & & &
\end{array}$$

Table I.4.1

$$
\begin{array}{c|cc|c|ccccc|c|ccc}
g_{0,1}^{(0)} & g_{0,2}^{(0)} & & & g_{0,r}^{(0)} & & & & & & g_{0,m}^{(0)} & & \\
 & & g_{1,2}^{(0)} & & & g_{1,r}^{(0)} & & & & & & \ddots & \\
g_{0,1}^{(1)} & g_{0,2}^{(1)} & & & g_{0,r}^{(1)} & & \ddots & & & & g_{0,m}^{(1)} & & \\
 & & g_{1,2}^{(1)} & & & g_{1,r}^{(1)} & & g_{r-1,r}^{(0)} & & & \vdots & & g_{m-1,m}^{(0)} \\
g_{0,1}^{(2)} & g_{0,2}^{(2)} & \vdots & \cdots & g_{0,r}^{(2)} & \vdots & & \vdots & & \cdots & & & \vdots \\
\vdots & \vdots & & & \vdots & & & g_{r-1,r}^{(n+m-r+1)} & & & & & g_{m-1,m}^{(n+1)} \\
 & & & & & & \cdot^{\cdot^{\cdot}} & & & & & & \\
 & & g_{1,2}^{(n+m-1)} & & & g_{1,r}^{(n+m-1)} & & & & & & \cdot^{\cdot^{\cdot}} & \\
g_{0,1}^{(n+m)} & g_{0,2}^{(n+m)} & & & g_{0,r}^{(n+m)} & & & & & & g_{0,m}^{(n+m)} & &
\end{array}
$$

Table I.4.2

We obtain

$$[N/D]_I = E_m^{(n)}$$

Since the solution $q(x, y)$ of $(I.3.1c)$ is unique, the value $E_m^{(n)}$ itself does not depend upon the numbering of the points within the sets N, D and H. But this numbering affects the interpolation conditions satisfied by the intermediate E-values.

THEOREM I.4.1. *For* $\ell = 0, ..., n$ *and* $r = 0, ..., m$

$$E_r^{(\ell)} = [N_\ell/D_r]_{N_\ell \cup \underbrace{\{(i_{\ell+1}, j_{\ell+1}), ..., (i_n, j_n), (h_1, k_1), ..., (h_{r-n+\ell}, k_{r-n+\ell})\}}_{r\ points}}$$

PROOF:: The proof is obvious since we know from [BREZb] that

$$E_r^{(\ell)} = \frac{\begin{vmatrix} t_0(\ell) & \dots & t_r(\ell) \\ \triangle\, t_0(\ell) & \dots & \triangle\, t_r(\ell) \\ \vdots & & \vdots \\ \triangle\, t_0(\ell + r - 1) & \dots & \triangle\, t_r(\ell + r - 1) \end{vmatrix}}{\begin{vmatrix} 1 & \dots & 1 \\ \triangle\, t_0(\ell) & \dots & \triangle\, t_r(\ell) \\ \vdots & & \vdots \\ \triangle\, t_0(\ell + r - 1) & \dots & \triangle\, t_r(\ell + r - 1) \end{vmatrix}}$$

and from [CUYTj] that

$$[N_\ell/D_r]_{N_\ell \cup \{(i_{\ell+1}, j_{\ell+1}), ..., (i_n, j_n), (h_1, k_1), ..., (h_{r-n+\ell}, k_{r-n+\ell})\}} =$$

$$= \frac{\begin{vmatrix} \sum_{(i,j) \in N_\ell} c_{d_0 i, e_0 j} B_{ij}(x, y) & \dots & \sum_{(i,j) \in N_\ell} c_{d_r i, e_r j} B_{ij}(x, y) \\ c_{d_0 i_{\ell+1}, e_0 j_{\ell+1}} & \dots & c_{d_r i_{\ell+1}, e_r j_{\ell+1}} \\ \vdots & & \vdots \end{vmatrix}}{\begin{vmatrix} B_{d_0 e_0}(x, y) & \dots & B_{d_r e_r}(x, y) \\ c_{d_0 i_{\ell+1}, e_0 j_{\ell+1}} & \dots & c_{d_r i_{\ell+1}, e_r j_{\ell+1}} \\ \vdots & & \vdots \end{vmatrix}}$$

If $n - \ell > r$ then the interpolation set does not contain points of H but only the points $\{(i_0, j_0), \ldots, (i_\ell, j_\ell), (i_{\ell+1}, j_{\ell+1}), \ldots, (i_r, j_r)\}$. ■

If N is enlarged with elements of H or if D is enlarged, then sufficient points of $\mathbb{N}^2$ should be added to I so that H is enlarged with the same number of points as N or D. The enumeration of the points in N, D and H can be adapted so that the first $(m+1)$ columns of the E-table remain unchanged and only subsequent columns or diagonals must be computed.

If N or D are completely changed, then it may be necessary to restart the algorithm.

If N and D contain the origin and satisfy the inclusion property themselves, then the structure of the g-table simplifies since

$$t_r(\ell) = 0 \qquad \ell = 0, \ldots, \frac{(d_r + e_r)(d_r + e_r + 1)}{2} + e_r - 1$$

We can tell from table I.4.3 that we get a band structure instead of a triangular table.

0			
$\vdots$	$\ddots$		
		0	
	$\cdot^{\cdot^{\cdot}}$		$g^{(0)}_{r-1,r}$
0			$\vdots$
		$\cdot^{\cdot^{\cdot}}$	
	$g^{(r-2)}_{1,r}$		$g^{(n+m-r+1)}_{r-1,r}$
$g^{(r-1)}_{0,r}$	$\vdots$	$\cdot^{\cdot^{\cdot}}$	
$\vdots$	$g^{(n+m-1)}_{1,r}$		
$g^{(n+m)}_{0,r}$			

Table I.4.3

5. Continued fraction representation and the qdg-algorithm.

Let us now suppose for the sake of simplicity that the homogeneous system of equations (I.3.3b) has maximal rank, in other words $H = I \backslash N$. As a consequence we have

$$\#I = n + m + 1$$

Hence we can write

$$I = \bigcup_{\ell=0}^{n+m} I_\ell$$

with

$$\begin{aligned} I_\ell &= N_\ell \qquad \ell = 0, \dots, n \\ I_{n+\ell} \backslash I_{n+\ell-1} &= \{(i_{n+\ell}, j_{n+\ell})\} \qquad \ell = 1, \dots, m \\ r(i_{n+\ell}, j_{n+\ell}) &> r(i_r, j_r) \qquad n + \ell > r \geq n + 1 \end{aligned}$$

With the subsets N_ℓ, D_r and $I_{\ell+r}$ rational interpolants

$$[N_\ell / D_r]_{I_{\ell+r}}$$

can be constructed which satisfy only part of the interpolation conditions and which are of lower "degree". To this end we assume that the numbering $r(i_r, j_r)$ of the points in $\mathbb{N}^2$ is such that the inclusion property of the set I is carried over to the subsets I_ℓ. With these functions we can fill up a table of rational interpolants :

$$\begin{array}{cccc} [N_0/D_0]_{I_0} & [N_0/D_1]_{I_1} & [N_0/D_2]_{I_2} & \dots \\ [N_1/D_0]_{I_1} & [N_1/D_1]_{I_2} & [N_1/D_2]_{I_3} & \dots \\ [N_2/D_0]_{I_2} & [N_2/D_1]_{I_3} & [N_2/D_2]_{I_4} & \dots \\ \vdots & \vdots & \vdots & \end{array}$$

Table I.5.1

where $[N/D]_I = [N_n/D_m]_{I_{n+m}}$. Our aim is to consider descending staircases of multivariate rational interpolants in table I.5.1

$$\begin{array}{llll} [N_s/D_0]_{I_s} & & & \\ [N_{s+1}/D_0]_{I_{s+1}} & [N_{s+1}/D_1]_{I_{s+2}} & & \\ & [N_{s+2}/D_1]_{I_{s+3}} & [N_{s+2}/D_2]_{I_{s+4}} & \\ & & \vdots & \ldots \end{array} \tag{I.5.1}$$

and construct continued fractions of which the ℓ^{th} convergent equals the ℓ^{th} interpolant on the staircase. We restrict ourselves to the case where every three successive elements in (I.5.1) are different. It is well-know that a continued fraction of which the ℓ^{th} convergent is the ℓ^{th} element of a given sequence $\{C_\ell\}_{\ell \in \mathbb{N}}$ with every three successive elements different from each other, is given by

$$C_0 + \left.\frac{C_1 - C_0}{1}\right| + \sum_{\ell=2}^{\infty} \left.\frac{\dfrac{C_{\ell-1} - C_\ell}{C_{\ell-1} - C_{\ell-2}}}{\dfrac{C_\ell - C_{\ell-2}}{C_{\ell-1} - C_{\ell-2}}}\right|$$

Let us compute the partial numerators and denominators of this continued fraction for the elements

$$C_{\ell+r} = [N_{\ell+s}/D_r]_{I_{\ell+r+s}} \qquad s \geq 0 \qquad \ell + r = 0, 1, 2, \ldots$$

on the descending staircase (I.5.1).

In the notation of the previous section we already have

$$C_0 = t_0(s) = \sum_{(i,j) \in N_s} c_{d_{0i}, e_{0j}} B_{d_{0i}, e_{0j}}(x, y)$$

$$C_1 - C_0 = \Delta t_0(s) = c_{d_0 i_{s+1}, e_0 j_{s+1}} B_{d_0 i_{s+1}, e_0 j_{s+1}}(x, y)$$

We shall now distinguish between even and odd numerators and denominators. For this purpose we introduce the notations

$$-q_\ell^{(s+1)} = \frac{C_{2\ell-1} - C_{2\ell}}{C_{2\ell-1} - C_{2\ell-2}}$$

$$-e_\ell^{(s+1)} = \frac{C_{2\ell} - C_{2\ell+1}}{C_{2\ell} - C_{2\ell-1}}$$

for the partial numerators. Consequently we can write for the partial denominators

$$1 + q_\ell^{(s+1)} = \frac{C_{2\ell} - C_{2\ell-2}}{C_{2\ell-1} - C_{2\ell-2}}$$

$$1 + e_\ell^{(s+1)} = \frac{C_{2\ell+1} - C_{2\ell-1}}{C_{2\ell} - C_{2\ell-1}}$$

In $q_\ell^{(s+1)}$ the convergents

$$\begin{array}{lll} \ldots & C_{2\ell-2} & \\ & C_{2\ell-1} & C_{2\ell} \\ & & \vdots \end{array}$$

of (I.5.1) are involved. In other words the rational interpolants

$$\begin{array}{lll} \ldots & [N_{\ell+s-1}/D_{\ell-1}]_{I_{2\ell+s-2}} & \\ & [N_{\ell+s}/D_{\ell-1}]_{I_{2\ell+s-1}} & [N_{\ell+s}/D_\ell]_{I_{2\ell+s}} \\ & & \vdots \end{array}$$

or, in the notation of the previous section,

$$\begin{array}{lll} \ldots & E_{\ell-1}^{(s+\ell-1)} & \\ & E_{\ell-1}^{(s+\ell)} & E_\ell^{(s+\ell)} \\ & & \vdots \end{array}$$

Hence, by using (I.4.2a)

$$\begin{aligned} q_\ell^{(s+1)} = \frac{C_{2\ell} - C_{2\ell-1}}{C_{2\ell-1} - C_{2\ell-2}} &= \frac{E_\ell^{(s+\ell)} - E_{\ell-1}^{(s+\ell)}}{E_{\ell-1}^{(s+\ell)} - E_{\ell-1}^{(s+\ell-1)}} \\ &= \frac{(E_{\ell-1}^{(s+\ell)} - E_{\ell-1}^{(s+\ell+1)})}{(E_{\ell-1}^{(s+\ell)} - E_{\ell-1}^{(s+\ell-1)})} \quad \frac{g_{\ell-1,\ell}^{(s+\ell)}}{g_{\ell-1,\ell}^{(s+\ell+1)} - g_{\ell-1,\ell}^{(s+\ell)}} \end{aligned} \tag{I.5.2}$$

In $e_\ell^{(s+1)}$ the convergents

$$\begin{array}{ccc} \vdots & & \\ C_{2\ell-1} & C_{2\ell} & \\ & C_{2\ell+1} & \dots \end{array}$$

of (I.5.1) are involved. In other words the rational interpolants

$$\begin{array}{ccc} \vdots & & \\ [N_{\ell+s}/D_{\ell-1}]_{I_{2\ell+s-1}} & [N_{\ell+s}/D_\ell]_{I_{2\ell+s}} & \\ & [N_{\ell+1+s}/D_\ell]_{I_{2\ell+1+s}} & \dots \end{array}$$

or the values

$$\begin{array}{ccc} \vdots & & \\ E_{\ell-1}^{(s+\ell)} & E_\ell^{(s+\ell)} & \\ & E_\ell^{(s+\ell+1)} & \dots \end{array}$$

In this way

$$e_\ell^{(s+1)} = \frac{C_{2\ell+1} - C_{2\ell}}{C_{2\ell} - C_{2\ell-1}} = \frac{E_\ell^{(s+\ell+1)} - E_\ell^{(s+\ell)}}{E_\ell^{(s+\ell)} - E_{\ell-1}^{(s+\ell)}} \qquad (I.5.3)$$

Combining (I.5.2) and (I.5.3) we find for $\ell \geq 2$

$$\begin{aligned} q_\ell^{(s+1)} &= e_{\ell-1}^{(s+2)} \quad \frac{(E_{\ell-2}^{(s+\ell)} - E_{\ell-1}^{(s+\ell)})}{(E_{\ell-1}^{(s+\ell)} - E_{\ell-1}^{(s+\ell-1)})} \quad \frac{g_{\ell-1,\ell}^{(s+\ell)}}{g_{\ell-1,\ell}^{(s+\ell+1)} - g_{\ell-1,\ell}^{(s+\ell)}} \\ &= -e_{\ell-1}^{(s+2)} q_{\ell-1}^{(s+2)} \quad \frac{(E_{\ell-2}^{(s+\ell)} - E_{\ell-2}^{(s+\ell-1)})}{(E_{\ell-1}^{(s+\ell)} - E_{\ell-1}^{(s+\ell-1)})} \quad \frac{g_{\ell-1,\ell}^{(s+\ell)}}{g_{\ell-1,\ell}^{(s+\ell+1)} - g_{\ell-1,\ell}^{(s+\ell)}} \\ &= \frac{-e_{\ell-1}^{(s+2)} q_{\ell-1}^{(s+2)}}{e_{\ell-1}^{(s+1)}} \quad \frac{(E_{\ell-2}^{(s+\ell)} - E_{\ell-2}^{(s+\ell-1)})}{(E_{\ell-1}^{(s+\ell-1)} - E_{\ell-2}^{(s+\ell-1)})} \quad \frac{g_{\ell-1,\ell}^{(s+\ell)}}{g_{\ell-1,\ell}^{(s+\ell+1)} - g_{\ell-1,\ell}^{(s+\ell)}} \\ &= \frac{e_{\ell-1}^{(s+2)} q_{\ell-1}^{(s+2)}}{e_{\ell-1}^{(s+1)}} \quad \frac{g_{\ell-2,\ell-1}^{(s+\ell)} - g_{\ell-2,\ell-1}^{(s+\ell-1)}}{g_{\ell-2,\ell-1}^{(s+\ell-1)}} \quad \frac{g_{\ell-1,\ell}^{(s+\ell)}}{g_{\ell-1,\ell}^{(s+\ell+1)} - g_{\ell-1,\ell}^{(s+\ell)}} \quad (I.5.4) \end{aligned}$$

and for $\ell \geq 1$

$$e_{\ell}^{(s+1)} + 1 = \frac{E_{\ell}^{(s+\ell+1)} - E_{\ell-1}^{(s+\ell)}}{E_{\ell}^{(s+\ell)} - E_{\ell-1}^{(s+\ell)}}$$

$$= -\frac{g_{\ell-1,\ell}^{(s+\ell+1)} - g_{\ell-1,\ell}^{(s+\ell)}}{g_{\ell-1,\ell}^{(s+\ell)}} \left(q_{\ell}^{(s+2)} + 1 \right) \qquad (I.5.5)$$

If we arrange the values $q_{\ell}^{(s+1)}$ and $e_{\ell}^{(s+1)}$ in a table as follows

$$\begin{array}{ccccc}
q_1^{(1)} & & & & \\
 & e_1^{(1)} & & & \\
q_1^{(2)} & & q_2^{(1)} & & \\
 & e_1^{(2)} & & e_2^{(1)} & \\
q_1^{(3)} & & q_2^{(2)} & & \ddots \\
 & e_1^{(3)} & & e_2^{(2)} & \\
q_1^{(4)} & & q_2^{(3)} & & \ddots \\
\vdots & e_1^{(4)} & \vdots & e_2^{(3)} & \\
 & \vdots & & \vdots &
\end{array}$$

Table I.5.2

where subscripts indicate columns and superscripts indicate downward sloping diagonals, then (I.5.4) links the elements in the rhombus

$$\begin{array}{ccc}
 & e_{\ell-1}^{(s+1)} & \\
q_{\ell-1}^{(s+2)} & & q_{\ell}^{(s+1)} \\
 & e_{\ell-1}^{(s+2)} &
\end{array}$$

and (I.5.5) links two elements on an upward sloping diagonal

$$\begin{array}{cc}
 & e_{\ell}^{(s+1)} \\
q_{\ell}^{(s+2)} &
\end{array}$$

If starting values for $q_\ell^{(s+1)}$ were known, all the values in table I.5.2 could be computed. These starting values are given by

$$q_1^{(s+1)} = \frac{E_1^{(s+1)} - E_0^{(s+1)}}{E_0^{(s+1)} - E_0^{(s)}} = \frac{-\Delta t_0(s+1)}{\Delta t_0(s)} \quad \frac{g_{0,1}^{(s+1)}}{g_{0,1}^{(s+2)} - g_{0,1}^{(s+1)}} \qquad (I.5.6)$$

Finally, we can say that, given a descending staircase (I.5.1) of different elements, it is possible to construct a continued fraction of the form

$$[N_s/D_0]_{I_s} + \frac{[N_{s+1}/D_0]_{I_{s+1}} - [N_s/D_0]_{I_s}\,|}{|\,1} + \frac{-q_1^{(s+1)}\,|}{|\,1+q_1^{(s+1)}} + \frac{-e_1^{(s+1)}\,|}{|\,1+e_1^{(s+1)}} + \frac{-q_2^{(s+1)}\,|}{|\,1+q_2^{(s+1)}} + \frac{-e_2^{(s+1)}\,|}{|\,1+e_2^{(s+1)}} + \ldots \qquad (I.5.7)$$

of which the successive convergents equal the successive elements on the descending staircase (I.5.1). Here

$$[N_s/D_0]_{I_s} = \sum_{(i,j)\in N_s} c_{d_0 i, e_0 j} B_{d_0 i, e_0 j}(x,y)$$

$$[N_{s+1}/D_0]_{I_{s+1}} = \sum_{(i,j)\in N_{s+1}} c_{d_0 i, e_0 j} B_{d_0 i, e_0 j}(x,y)$$

and the coefficients $q_\ell^{(s+1)}$ and $e_\ell^{(s+1)}$ can be computed using (I.5.4-6).

In analogy with the univariate Padé approximation case [HENR p. 610] and the univariate rational Hermite interpolation case [CLAEa] it is also possible to give explicit determinant formulas for the partial numerators in (I.5.7). Let us introduce the notations

$$H_0(h,k) = \begin{vmatrix} \Delta t_0(h) & \ldots & \Delta t_{k-1}(h) \\ \vdots & & \vdots \\ \Delta t_0(h+k-1) & \ldots & \Delta t_{k-1}(h+k-1) \end{vmatrix} \qquad H_0(h,0) = 0$$

$$H_1(h,k) = \begin{vmatrix} 1 & \ldots & 1 \\ \Delta t_0(h) & \ldots & \Delta t_k(h) \\ \vdots & & \vdots \\ \Delta t_0(h+k-1) & \ldots & \Delta t_k(h+k-1) \end{vmatrix} \qquad H_1(h,-1) = 0$$

$$H_2(h,k) = \begin{vmatrix} t_0(h) & \dots & t_k(h) \\ \triangle\, t_0(h) & \dots & \triangle\, t_k(h) \\ \vdots & & \vdots \\ \triangle\, t_0(h+k-1) & \dots & \triangle\, t_k(h+k-1) \end{vmatrix} \qquad H_2(h,-1)=0$$

$$H_3(h,k) = \begin{vmatrix} 1 & \dots & 1 \\ t_0(h) & \dots & t_k(h) \\ \triangle\, t_0(h) & \dots & \triangle\, t_k(h) \\ \vdots & & \vdots \\ \triangle\, t_0(h+k-2) & \dots & \triangle\, t_k(h+k-2) \end{vmatrix} \qquad H_3(h,-1)=0$$

We know from (I.3.5) that

$$\frac{H_2(h,k)}{H_1(h,k)} = [N_h/D_k]_{I_{h+k}}$$

Besides the differences $\triangle t_r(\ell)$ we can also consider

$$\delta t_r(\ell) = t_{r+1}(\ell) - t_r(\ell)$$

and introduce the notations

$$G_0(h,k) = \begin{vmatrix} \delta t_0(h) & \dots & \delta t_0(h+k-1) \\ \vdots & & \vdots \\ \delta t_{k-1}(h) & \dots & \delta t_{k-1}(h+k-1) \end{vmatrix} \qquad G_0(h,0)=0$$

$$G_1(h,k) = \begin{vmatrix} 1 & \dots & 1 \\ \delta t_0(h) & \dots & \delta t_0(h+k) \\ \vdots & & \vdots \\ \delta t_{k-1}(h) & \dots & \delta t_{k-1}(h+k) \end{vmatrix} \qquad G_1(h,-1)=0$$

$$G_2(h,k) = \begin{vmatrix} t_0(h) & \dots & t_0(h+k) \\ \delta t_0(h) & \dots & \delta t_0(h+k) \\ \vdots & & \vdots \\ \delta t_{k-1}(h) & \dots & \delta t_{k-1}(h+k) \end{vmatrix} \qquad G_2(h,-1)=0$$

$$G_3(h,k) = \begin{vmatrix} 1 & \dots & 1 \\ t_0(h) & \dots & t_0(h+k) \\ \delta t_0(h) & \dots & \delta t_0(h+k) \\ \vdots & & \vdots \\ \delta t_{k-2}(h) & \dots & \delta t_{k-2}(h+k) \end{vmatrix} \qquad G_3(h,-1) = 0$$

For the H-values it is well-known by the Schweins expansion [BREZa p. 43] that

$$H_1(h,k)H_2(h,k-1) - H_1(h,k-1)H_2(h,k) = H_3(h,k)H_0(h,k) \quad (I.5.8)$$

For the G-values one can prove using the Sylvester-identity that

$$G_1(h-1,k)G_2(h,k) - G_1(h,k)G_2(h-1,k) = G_3(h-1,k+1)G_0(h,k) \quad (I.5.9)$$

$$G_1(h-1,k)G_0(h,k+1) - G_1(h,k)G_0(h-1,k+1) = G_1(h-1,k+1)G_0(h,k) \quad (I.5.10)$$

Some easy computations show that the G-values are very related to the H-values. For $k \geq 1$ we have

$$H_0(h,k) = G_3(h,k)$$
$$H_3(h,k) = G_0(h,k)$$

and for $k \geq 0$

$$H_1(h,k) = G_1(h,k)$$
$$H_2(h,k) = G_2(h,k)$$

Hence we know from (I.5.8) and (I.5.9) that also

$$G_1(h,k)G_2(h,k-1) - G_1(h,k-1)G_2(h,k) = G_0(h,k)G_3(h,k) \quad (I.5.11)$$

and that for $k \geq 1$

$$H_1(h-1,k)H_2(h,k) - H_1(h,k)H_2(h-1,k) = H_0(h-1,k+1)H_3(h,k) \quad (I.5.12)$$

By means of these formulas we can prove the following theorem.

THEOREM I.5.1. *For the partial numerators $q_\ell^{(s+1)}$ and $e_\ell^{(s+1)}$ in the continued fraction (I.5.7) of which the successive convergents equal the successive elements on the descending staircase (I.5.1), the following determinant formulas hold:*

$$q_\ell^{(s+1)} = -\frac{H_0(s+\ell,\ell)H_1(s+\ell-1,\ell-1)H_3(s+\ell,\ell)}{H_0(s+\ell-1,\ell)H_1(s+\ell,\ell)H_3(s+\ell,\ell-1)} \qquad (I.5.13)$$

$$e_\ell^{(s+1)} = -\frac{H_0(s+\ell,\ell+1)H_1(s+\ell,\ell-1)H_3(s+\ell+1,\ell)}{H_0(s+\ell,\ell)H_1(s+\ell+1,\ell)H_3(s+\ell,\ell)} \qquad (I.5.14)$$

PROOF: We know from (I.5.2) and theorem I.4.1 that

$$q_\ell^{(s+1)} = \frac{E_\ell^{(s+\ell)} - E_{\ell-1}^{(s+\ell)}}{E_{\ell-1}^{(s+\ell)} - E_{\ell-1}^{(s+\ell-1)}}$$

$$= \frac{\dfrac{H_2(s+\ell,\ell)}{H_1(s+\ell,\ell)} - \dfrac{H_2(s+\ell,\ell-1)}{H_1(s+\ell,\ell-1)}}{\dfrac{H_2(s+\ell,\ell-1)}{H_1(s+\ell,\ell-1)} - \dfrac{H_2(s+\ell-1,\ell-1)}{H_1(s+\ell-1,\ell-1)}}$$

Using (I.5.8) and (I.5.12) we get

$$q_\ell^{(s+1)} = -\frac{H_3(s+\ell,\ell)H_0(s+\ell,\ell)}{H_1(s+\ell,\ell)H_1(s+\ell,\ell-1)} \Big/ \frac{H_0(s+\ell-1,\ell)H_3(s+\ell,\ell-1)}{H_1(s+\ell,\ell-1)H_1(s+\ell-1,\ell-1)}$$

$$= -\frac{H_0(s+\ell,\ell)H_1(s+\ell-1,\ell-1)H_3(s+\ell,\ell)}{H_0(s+\ell-1,\ell)H_1(s+\ell,\ell)H_3(s+\ell,\ell-1)}$$

The formula for $e_\ell^{(s+1)}$ is proved in a completely analogous way. ∎

Note that one can prove, using (I.5.9) and (I.5.10) that

$$\frac{H_2(h,k)}{H_1(h,k)} = E_k^{(h)} = \frac{G_2(h,k)}{G_1(h,k)}$$

$$= \frac{\dfrac{G_2(h,k-1)}{G_1(h,k-1)}\dfrac{G_0(h+1,k)}{G_1(h+1,k-1)} - \dfrac{G_2(h+1,k-1)}{G_1(h+1,k-1)}\dfrac{G_0(h,k)}{G_1(h,k-1)}}{\dfrac{G_0(h+1,k)}{G_1(h+1,k-1)} - \dfrac{G_0(h,k)}{G_1(h,k-1)}}$$

$$= \frac{E_{k-1}^{(h)}\dfrac{G_0(h+1,k)}{G_1(h+1,k-1)} - E_{k-1}^{(h+1)}\dfrac{G_0(h,k)}{G_1(h,k-1)}}{\dfrac{G_0(h+1,k)}{G_1(h+1,k-1)} - \dfrac{G_0(h,k)}{G_1(h,k-1)}}$$

Referring to (I.4.2a) we see that

$$\frac{G_0(h+1,k)}{G_1(h+1,k-1)} = g_{k-1,k}^{(h+1)}$$
$$\frac{G_0(h,k)}{G_1(h,k-1)} = g_{k-1,k}^{(h)}$$

Obviously the formulas from section 4, involving recursive computation and those of section 5, involving continued fraction representation, are closely linked. This is to be expected if we want to develop a multivariate theory with the properties of the univariate theory.

6. SPECIAL CASES.

This multivariate theory, in which a rational interpolant can be obtained explicitly by means of the formulas (I.3.5) or by its values via the algorithm (I.4.2) or as a convergent of the continued fraction (I.5.7), includes a number of interesting special cases.

(a) Univariate rational interpolants of degree n in the numerator and m in the denominator can be obtained by choosing

$$D = \{(d,0) \mid 0 \le d \le m\}$$

$$N = \{(i,0) \mid 0 \le i \le n\}$$

$$H \subset I \backslash N = \{(h,0) \mid n+1 \le h \le n+m+s, \quad s \ge 0\}$$

where the integer s is the number of linearly dependent interpolation conditions in $I\backslash N$. The E-algorithm then simplifies to an ε-like algorithm [CLAEd, CUYTj] and the qdg-algorithm simplifies to the generalized qd-algorithm [CLAEa].

(b) As a consequence of the previous remark univariate Padé approximants also result as a special case by letting all the interpolation points coincide in the univariate formulation. The E-algorithm now reduces to Wynn's ε-algorithm [WYNN] and the qdg-algorithm to Rutishauser's qd-algorithm [HENR].

(c) The multivariate Padé approximants of order (ν, μ) introduced in [CUYTd, CUYTf], which prove to satisfy a large number of the classical univariate properties, can already be calculated recursively by means of the ε-algorithm [CUYTg] and can also be represented in continued fraction form using the qd-algorithm [CUYTi]. To this end the $\Delta t_r(\ell-1)$ and $\Delta t_r(n+\ell-1)$ are homogeneous forms af degree $\ell - r$ and $n+\ell-r$ respectively given by

$$\Delta t_r(\ell - 1) = \sum_{i+j=\ell-r} c_{0i,0j} B_{ij}(x,y)$$

$$\Delta t_r(n+\ell-1) = \sum_{i+j=n+\ell-r} c_{0i,0j} B_{ij}(x,y)$$

where

$$c_{0i,0j} = \frac{1}{i!}\frac{1}{j!}\frac{\partial^{i+j} f}{\partial x^i \partial y^j}\,|_{(0,0)}$$

These approximants can now be obtained by following a different approach and the computations can be performed in a different way by constructing Δt_r as described in section 4. To this end we choose

$$D = \{(d,e) \mid nm \le d+e \le nm+m\}$$

$$N = \{(i,j) \mid nm \le i+j \le nm+n\}$$

$$H \subset \{(h,k) \mid nm \le h+k \le nm+n+m+s, \quad s \ge 0\}$$

where the integer s is related to the block-size of this multivariate Padé table. For more details see [CUYTb]. Explicit determinant formulas for these index sets, involving near-Toeplitz matrices, are given in [CUYTb]. The case $s=0$ and $H = I \backslash N$ is treated in more detail further on.

(d) Last but not least, a great number of multivariate Padé approximants defined in the last decade, can now also be computed recursively and represented in continued fraction form by letting the multivariate interpolation points, used in the previous sections, coincide with the origin. The basisfunctions and divided differences become

$$B_{ki,lj}(x,y) = x^{i-k} y^{j-l}$$

$$c_{ki,lj} = \frac{\partial^{i-k+j-l} f}{\partial x^{i-k} \partial y^{j-l}}\,|_{(0,0)}$$

We shall consider here all types of definitions based on the use of a linear system of defining equations for the numerator and denominator coefficients of the multivariate Padé approximant. Definitions of this type can be found in [CHISc, CUYTd, HUGH, KARL, LEVIa, LUTTa, LUTTb]. The framework used to describe this group of definitions, is greatly inspired by [LEVIa].

Given a Taylor series expansion

$$f(x,y) = \sum_{(i,j)\in \mathbb{N}^2} c_{0i,0j} x^i y^j$$

with

$$\ddot{c}_{0i,0j} = \frac{1}{i!}\frac{1}{j!}\frac{\partial^{i+j} f}{\partial x^i \partial y^j}\,|_{(0,0)}$$

we shall compute an approximant $p(x,y)/q(x,y)$ to $f(x,y)$ where $p(x,y)$ and $q(x,y)$ are determined by the accuracy–through–order principle. The polynomials $p(x,y)$ and $q(x,y)$ are of the form

$$p(x,y) = \sum_{(i,j)\in N} a_{ij} x^i y^j$$

$$q(x,y) = \sum_{(i,j)\in D} b_{ij} x^i y^j$$

where N and D are finite subsets of $I\!N^2$. The sets N and D indicate the degree of the polynomials $p(x,y)$ and $q(x,y)$. Let us denote

$$\#N = n+1$$

$$\#D = m+1$$

It is now possible to let $p(x,y)$ and $q(x,y)$ satisfy the following condition for the power series $(fq-p)(x,y)$, namely

$$(fq-p)(x,y) = \sum_{(i,j)\in I\!N^2\setminus I} d_{ij} x^i y^j \qquad (I.6.1)$$

if, in analogy with the univariate case, the index set I is such that

$$N \subseteq I \qquad (I.6.2a)$$

$$\#(I\setminus N) = m = \#D - 1 \qquad (I.6.2b)$$

I satisfies the inclusion property $\qquad (I.6.2c)$

meaning that when a point belongs to the index set I, then the rectangular subset of points emanating from the origin with the given point as its furthermost corner, also lies in I. Condition (I.6.2a) enables us to split the system of equations

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

in an inhomogeneous part defining the numerator coefficients

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

and a homogeneous part defining the denominator coefficients

$$\sum_{\mu=0}^{i}\sum_{\nu=0}^{j} c_{0\mu,0\nu} b_{i-\mu,j-\nu} = 0 \qquad (i,j) \in I\backslash N \qquad (I.6.3)$$

By convention

$$b_{k\ell} = 0 \qquad (k,\ell) \notin D$$

Condition (I.6.2b) 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 (I.6.2c) finally takes care of the Padé approximation property, namely

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

For more information we refer to [CUYTc, CUYTd].

For the sake of simplicity we assume that the homogeneous system of equations (I.6.3) has maximal rank. From numerical experiments we know that this is most often the case. However, what follows can be extended to the case when this is not true, by adding points to the set $I\backslash N$ until the rank deficiency has disappeared, but at this moment this would only complicate the notations. Using the numbering $r(i,j)$ of the points in $\mathbb{N}^2$, based on the enumeration given in section 4, we can write

$$N = \bigcup_{\ell=0}^{n} N_\ell$$

$$D = \bigcup_{\ell=0}^{m} D_\ell$$

$$I = N \cup \left(\bigcup_{\ell=n+1}^{n+m} I_\ell \right)$$

where N_ℓ, D_ℓ and I_ℓ are defined as in the sections 4 and 5. It was shown in [LEVIa] that a determinant representation for

$$p_h(x,y) = \sum_{(i,j)\in N_h} a_{ij} x^i y^j \qquad 0 \le h \le n$$

and

$$q_k(x,y) = \sum_{(i,j)\in D_k} b_{ij} x^i y^j \qquad 0 \le k \le m$$

satisfying

$$(fq_k - p_h)(x,y) = \sum_{(i,j)\in \mathbb{N}^2 \setminus I_{h+k}} d_{ij} x^i y^j$$

is given by

$$p_h(x,y) = \begin{vmatrix} \sum_{(i,j)\in N_h} c_{i-d_0,j-e_0} x^i y^j & \cdots & \sum_{(i,j)\in N_h} c_{i-d_k,j-e_k} x^i y^j \\ c_{i_{h+1}-d_0,j_{h+1}-e_0} & \cdots & c_{i_{h+1}-d_k,j_{h+1}-e_k} \\ \vdots & & \vdots \\ c_{i_{h+k}-d_0,j_{h+k}-e_0} & \cdots & c_{i_{h+k}-d_k,j_{h+k}-e_k} \end{vmatrix} \tag{I.6.4a}$$

$$q_k(x,y) = \begin{vmatrix} x^{d_0} y^{e_0} & \cdots & x^{d_k} y^{e_k} \\ c_{i_{h+1}-d_0,j_{h+1}-e_0} & \cdots & c_{i_{h+1}-d_k,j_{h+1}-e_k} \\ \vdots & & \vdots \\ c_{i_{h+k}-d_0,j_{h+k}-e_0} & \cdots & c_{i_{h+k}-d_k,j_{h+k}-e_k} \end{vmatrix} \tag{I.6.4b}$$

where

$$c_{0i,0j} = 0 \qquad i < 0 \quad \text{or} \quad j < 0$$

A solution of the original problem (I.6.1) is then given by

$$\frac{p_n(x,y)}{q_m(x,y)}$$

because

$$\begin{aligned} N_n &= N \\ D_m &= D \\ I_{n+m} &= I \end{aligned}$$

In order to show that this general setting can handle quite a number of previously given definitions of multivariate Padé approximations, we shall now give the sets N,D and I for several of these definitions.

When we are dealing with Karlsson-Wallin [KARL] Padé approximants, we must choose ν and μ in $I\!N$ and construct

$$N = \{(i,j) \in I\!N^2 \mid 0 \leq i+j \leq \nu\}$$

$$D = \{(d,e) \in I\!N^2 \mid 0 \leq d+e \leq \mu\}$$

which are triangular sets. In this way

$$\#N = n+1 = \frac{1}{2}(\nu+1)(\nu+2)$$

$$\#D = m+1 = \frac{1}{2}(\mu+1)(\mu+2)$$

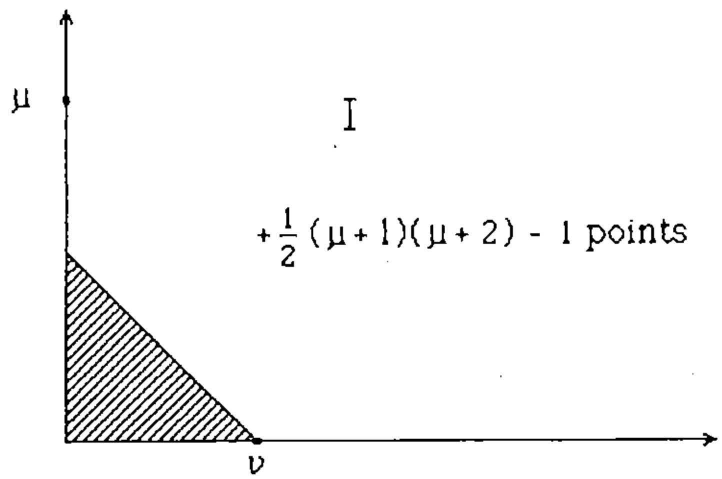

Figure I.6.1

For Padé approximants introduced by Lutterodt [LUTTb], we have with $\nu_1, \nu_2, \mu_1, \mu_2$ fixed

$$N = \{(i,j) \in I\!N^2 \mid 0 \le i \le \nu_1,\ 0 \le j \le \nu_2\}$$

$$D = \{(d,e) \in I\!N^2 \mid 0 \le d \le \mu_1,\ 0 \le e \le \mu_2\}$$

which are rectangular sets. Now

$$\#N = n + 1 = (\nu_1 + 1)(\nu_2 + 1)$$

$$\#D = m + 1 = (\mu_1 + 1)(\mu_2 + 1)$$

For these two types of multivariate Padé approximants, the only demands for the set I are the conditions (I.6.2a–c).

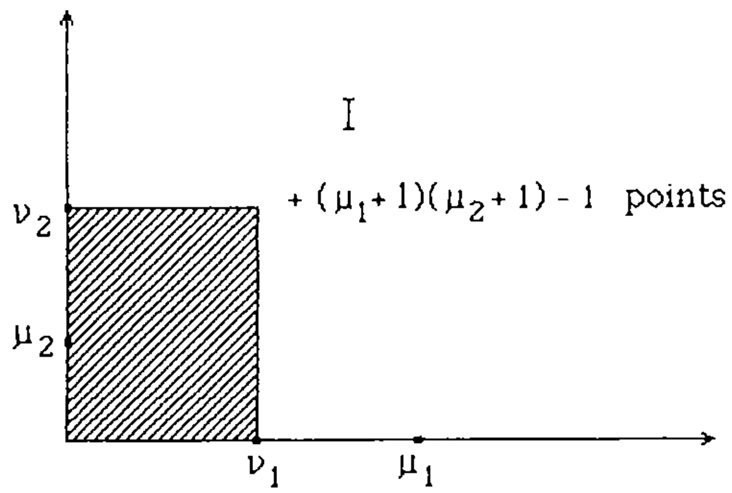

Figure I.6.2

Multivariate Padé approximants of order (ν, μ) introduced by Cuyt [CUYTd] appear to have numerator and denominator index sets given by

$$N = \{(i,j) \in I\!N^2 \mid \nu\mu \le i + j \le \nu\mu + \nu\}$$

$$D = \{(d,e) \in I\!N^2 \mid \nu\mu \le d + e \le \nu\mu + \mu\}$$

which resemble triangular sets. Here

$$
\begin{aligned}
I &= I_1 \cup I_2 \\
I_1 &= \{(i,j) \in \mathbb{N}^2 \mid \nu\mu \le i+j \le \nu\mu+\nu+\mu\} \\
I_2 &= \{(i,j) \in \mathbb{N}^2 \mid 0 \le i+j < \nu\mu\}
\end{aligned}
$$

where the conditions in I_2 are automatically satisfied by the choices of N and D.

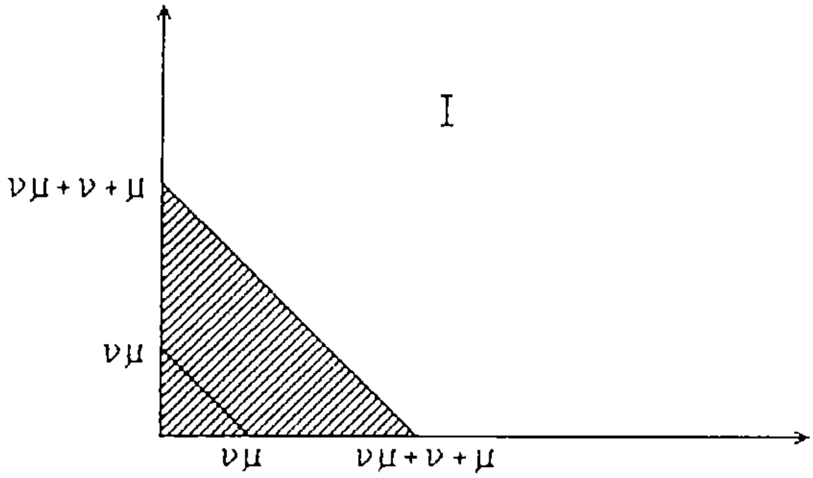

Figure I.6.3

The approximants introduced by the group working in Canterbury [CHISc, HUGH] were constructed from

$$
\begin{aligned}
N &= \{(i,j) \in \mathbb{N}^2 \mid 0 \le i \le \nu_1,\ 0 \le j \le \nu_2\} \\
D &= \{(d,e) \in \mathbb{N}^2 \mid 0 \le d \le \mu_1,\ 0 \le e \le \mu_2\} \\
I &= N \cup D \cup I_1 \cup I_2
\end{aligned}
$$

with

$$
\begin{aligned}
I_1 = \{(i,j) \in \mathbb{N}^2 \mid\ & 0 \le j \le \min(\nu_2,\mu_2), \\
& \max(\nu_1,\mu_1) < i \le \nu_1+\mu_1,\ i+j \le \nu_1+\mu_1\} \\
I_2 = \{(i,j) \in \mathbb{N}^2 \mid\ & 0 \le i \le \min(\nu_1,\mu_1), \\
& \max(\nu_2,\mu_2) < j \le \nu_2+\mu_2,\ i+j \le \nu_2+\mu_2\}
\end{aligned}
$$

with the additional requirements

$$d_{\nu_1+\mu_1+1-\ell,\ell} + d_{\ell,\nu_2+\mu_2+1-\ell} = 0 \qquad \ell = 1, \ldots, \min(\nu_1, \mu_1, \nu_2, \mu_2)$$

These additional requirements alter the determinant representations (I.6.4a) and (I.6.4b) but the structure of the determinants remains the same. For more details we refer to [LEVIa].

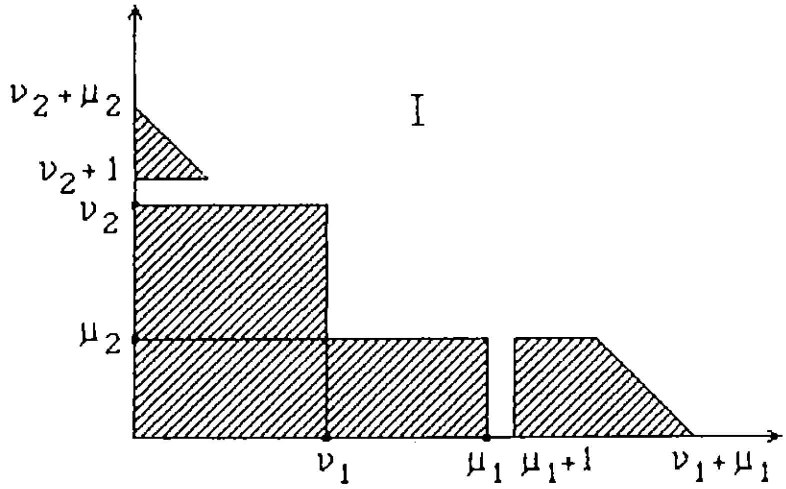

Figure I.6.4

For all these definitions the determinant formulas (I.6.4) can be rewritten as

$$p_h(x,y) = \begin{vmatrix} t_0(h) & \ldots & t_k(h) \\ \Delta\, t_0(h) & \ldots & \Delta\, t_k(h) \\ \vdots & & \vdots \\ \Delta\, t_0(h+k-1) & \ldots & \Delta\, t_k(h+k-1) \end{vmatrix} \qquad (I.6.5a)$$

$$q_k(x,y) = \begin{vmatrix} 1 & \ldots & 1 \\ \Delta\, t_0(h) & \ldots & \Delta\, t_k(h) \\ \vdots & & \vdots \\ \Delta\, t_0(h+k-1) & \ldots & \Delta\, t_k(h+k-1) \end{vmatrix} \qquad (I.6.5b)$$

This quotient of determinants can again be computed using the E-algorithm given in (I.4.2) if the series $t_0, \ldots, t_k$ are defined as in section4, but now using Taylor coefficients instead of divided differences:

$$t_0(0) = c_{0\ i_0-d_0,0\ j_0-e_0} x^{i_0-d_0} y^{j_0-e_0}$$

$$\Delta t_0(\ell-1) = t_0(\ell) - t_0(\ell-1) = c_{0\ i_\ell-d_0,0\ j_\ell-e_0} x^{i_\ell-d_0} y^{j_\ell-e_0} \qquad \ell = 1, \ldots, h+k \qquad (I.6.6a)$$

$$\Delta t_0(\ell-1) = 0 \qquad i_\ell < d_0 \text{ or } j_\ell < e_0$$

$$t_r(0) = c_{0\ i_0-d_r,0\ j_0-e_r} x^{i_0-d_r} y^{j_0-e_r}$$

$$\Delta t_r(\ell-1) = t_r(\ell) - t_r(\ell-1) = c_{i_\ell-d_r, j_\ell-e_r} x^{i_\ell-d_r} y^{j_\ell-e_r} \qquad \ell = 1, \ldots, h+k \qquad (I.6.6b)$$

$$\Delta t_r(\ell-1) = 0 \qquad i_\ell < d_r \text{ or } j_\ell < e_r$$

Finally with $h = n$ and $k = m$, this is with $N_h = N$, $D_k = D$ and $I_{h+k} = I$ we get

$$\frac{p_n(x,y)}{q_m(x,y)} = E_m^{(n)}$$

while intermediate values in the computation scheme are also multivariate Padé approximants since

$$E_k^{(h)} = \frac{p_h(x,y)}{q_k(x,y)}$$

and thus

$$f - E_k^{(h)} = \sum_{(i,j)\in \mathbb{N}^2 \setminus I_{h+k}} e_{ij} x^i y^j$$

In the same way as in section 5, these intermediate values can be used to build a table of multivariate Padé approximants:

$$\begin{array}{cccc}
[N_0/D_0]_{I_0} & [N_0/D_1]_{I_1} & [N_0/D_2]_{I_2} & \dots \\
[N_1/D_0]_{I_1} & [N_1/D_1]_{I_2} & [N_1/D_2]_{I_3} & \dots \\
[N_2/D_0]_{I_2} & [N_2/D_1]_{I_3} & [N_2/D_2]_{I_4} & \dots \\
\vdots & \vdots & \vdots &
\end{array}$$

Table I.6.1

Using the formulas (I.5.4), (I.5.5) and (I.5.6) again continued fractions of the form (I.5.7) can be constructed of which the successive convergents are the multivariate Padé approximants on the descending staircase

$$\begin{array}{llll}
[N_s/D_0]_{I_s} & & & \\
[N_{s+1}/D_0]_{I_{s+1}} & [N_{s+1}/D_1]_{I_{s+2}} & & \\
& [N_{s+2}/D_1]_{I_{s+3}} & [N_{s+2}/D_2]_{I_{s+4}} & \\
& & \vdots & \dots
\end{array} \qquad (I.5.1)$$

For the starting values

$$q_1^{(s+1)} = \frac{-\Delta t_0(s+1)}{\Delta t_0(s)} \quad \frac{g_{0,1}^{(s+1)}}{g_{0,1}^{(s+2)} - g_{0,1}^{(s+1)}} \qquad (I.6.7)$$

the series t_0 is defined as in (I.6.6a). The determinant formulas (I.5.13) and (I.5.14) remain valid as well with t_r defined as in (I.6.6b). So we see that Padé approximants originally only introduced via defining equations, can be given via a recursive scheme and can be obtained as the convergent of a multivariate continued fraction. In this way the univariate equivalence of the three main defining techniques for Padé approximants is also established for the multivariate case: algebraic relations, recurrence relations, continued fractions.

1. APPROXIMATION OF FUNCTIONS.

Let us illustrate a number of all these rational interpolants and approximants by some numerical results. When we are dealing with interpolation problems, we must specify whether we are interested in an explicit formula for the interpolant or only in its value at some points different from the interpolation points. The former gives rise to a **coefficient problem** while the latter is a **value problem**. Suppose we have to solve the following numerical problem. A bivariate function $f(x,y)$ is only known by its function values in a number of distinct points (x_i, y_j) and we need an approximation for the value of f in some other points (u_i, v_j). This problem can be solved by calculating the function value of an interpolatory function (polynomial or rational) with or without solving the coefficient problem. The bivariate Beta function $B(x,y)$ will serve as a concrete example here. It is defined by

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

where Γ is the Gamma function. Singularities occur 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

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

We shall now compute several types of approximants $R(x,y)$ for $f(x-1, y-1)$ and compare the exact value $B(u_i, v_j)$ with the expression

$$\frac{1 + (u_i - 1)(v_j - 1)R(u_i, v_j)}{u_i v_j}$$

Let us use the following interpolation methods:

(a) Polynomial interpolation

$$R(x,y)=\sum_{i=0}^{n_1}\sum_{j=0}^{n_2} f[x_0,\ldots,x_i][y_0,\ldots,y_j]B_{ij}(x,y)$$

satisfying

$$(f-R)(x,y)=\sum_{\{(i,j)|i>n_1 \text{ or } j>n_2\}} c_{ij}B_{ij}(x,y)$$

(b) Symmetric branched continued fractions of the form [CUYTk]

$$R(x,y)=\varphi[x_0][y_0]+\sum_{k=1}^{n_{0,x}}\frac{x-x_{k-1}|}{|\varphi[x_0,\ldots,x_k][y_0]}+\sum_{k=1}^{n_{0,y}}\frac{y-y_{k-1}|}{|\varphi[x_0][y_0,\ldots,y_k]}+$$

$$+\sum_{\ell=1}^{n}\frac{(x-x_{\ell-1})(y-y_{\ell-1})|}{|\varphi[x_0,\ldots,x_\ell][y_0,\ldots,y_\ell]+\sum_{k=\ell+1}^{n_{\ell x}}\frac{x-x_{k-1}|}{|\varphi[x_0,\ldots,x_k][y_0,\ldots,y_\ell]}+\sum_{k=\ell+1}^{n_{\ell y}}\frac{y-y_{k-1}|}{|\varphi[x_0,\ldots,x_\ell][y_0,\ldots,y_k]}}$$

where

$$\varphi[x_0][y_0]=f(x_0,y_0)$$

$$\varphi[x_0,\ldots,x_k][y_0]=\frac{x_k-x_{k-1}}{\varphi[x_0,\ldots,x_{k-2},x_k][y_0]-\varphi[x_0,\ldots,x_{k-2},x_{k-1}][y_0]}$$

$$\varphi[x_0][y_0,\ldots,y_k]=\frac{y_k-y_{k-1}}{\varphi[x_0][y_0,\ldots,y_{k-2},y_k]-\varphi[x_0][y_0,\ldots,y_{k-2},y_{k-1}]}$$

$$\varphi[x_0,\ldots,x_\ell][y_0,\ldots,y_\ell]=$$

$$\frac{(x_\ell-x_{\ell-1})(y_\ell-y_{\ell-1})}{\begin{array}{c}\varphi[x_0,\ldots,x_{\ell-2},x_\ell][y_0,\ldots,y_{\ell-2},y_\ell]-\varphi[x_0,\ldots,x_{\ell-2},x_{\ell-1}][y_0,\ldots,y_{\ell-2},y_\ell]\\ -\varphi[x_0,\ldots,x_{\ell-2},x_\ell][y_0,\ldots,y_{\ell-2},y_{\ell-1}]+\varphi[x_0,\ldots,x_{\ell-2},x_{\ell-1}][y_0,\ldots,y_{\ell-2},y_{\ell-1}]\end{array}}$$

and for $k > \ell$

$$\varphi[x_0, \ldots, x_k][y_0, \ldots, y_\ell] = \frac{x_k - x_{k-1}}{\varphi[x_0, \ldots, x_{k-2}, x_k][y_0, \ldots, y_\ell] - \varphi[x_0, \ldots, x_{k-2}, x_{k-1}][y_0, \ldots, y_\ell]}$$

$$\varphi[x_0, \ldots, x_\ell][y_0, \ldots, y_k] = \frac{y_k - y_{k-1}}{\varphi[x_0, \ldots, x_\ell][y_0, \ldots, y_{k-2}, y_k] - \varphi[x_0, \ldots, x_\ell][y_0, \ldots, y_{k-2}, y_{k-1}]}$$

satisfying

$$(f - R)(x, y) = \sum_{\substack{\mathbb{N}^2 \setminus \{(i,j) | 0 \le i \le n\,,\, 0 \le j \le n_{iy}\} \\ \setminus \{(j,i) | 0 \le i \le n\,,\, 0 \le j \le n_{ix}\}}} c_{ij} B_{ij}(x; y)$$

(c) Branched continued fractions of the form [SIEM]

$$R(x; y) = \psi[x_0][y_0] + \sum_{k=1}^{n_0} \left| \frac{y - y_{k-1}}{\psi[x_0][y_0, \ldots, y_k]} \right. + \sum_{\ell=1}^{n} \left| \frac{x - x_{\ell-1}}{\psi[x_0, \ldots, x_\ell][y_0] + \sum_{k=1}^{n_\ell} \left| \frac{y - y_{k-1}}{\psi[x_0, \ldots, x_\ell][y_0, \ldots, y_k]} \right.} \right.$$

with

$$\psi[x_0][y_0] = f(x_0, y_0)$$

$$\psi[x_0][y_0, \ldots, y_k] = \frac{y_k - y_{k-1}}{\psi[x_0][y_0, \ldots, y_{k-2}, y_k] - \psi[x_0][y_0, \ldots, y_{k-2}, y_{k-1}]}$$

$$\psi[x_0, \ldots, x_\ell][y_0] = \frac{x_\ell - x_{\ell-1}}{\psi[x_0, \ldots, x_{\ell-2}, x_\ell][y_0] - \psi[x_0, \ldots, x_{\ell-2}, x_{\ell-1}][y_0]}$$

and for $\ell \geq 1$

$$\psi[x_0, \ldots, x_\ell][y_0, \ldots, y_k] = \frac{y_k - y_{k-1}}{\psi[x_0, \ldots, x_\ell][y_0, \ldots, y_{k-2}, y_k] - \psi[x_0, \ldots, x_\ell][y_0, \ldots, y_{k-2}, y_{k-1}]}$$

satisfying

$$(f-R)(x,y) = \sum_{\mathbb{N}^2 \setminus \{(i,j) \mid 0 \le i \le n\,,\, 0 \le j \le n_i\}} c_{ij} B_{ij}(x,y)$$

(d) Multivariate Padé approximants calculated by means of the ε-algorithm [CUYTg]

$$R(x,y) = \varepsilon_{2m}^{(n-m)}$$

with

$$\varepsilon_{-1}^{(k)} = 0 \qquad k = 0, 1, \ldots$$

$$\varepsilon_0^{(k)} = \sum_{i+j=0}^{k} \frac{1}{i!j!} \frac{\partial^{i+j} f}{\partial x^i \partial y^j} \Big|_{(0,0)} x^i y^j \qquad k = 0, \ldots, n+m$$

$$\varepsilon_{2\ell}^{(-\ell-1)} = 0 \qquad \ell = 0, 1, \ldots$$

$$\varepsilon_{\ell+1}^{(k)} = \varepsilon_{\ell-1}^{(k+1)} + \frac{1}{\varepsilon_\ell^{(k+1)} - \varepsilon_\ell^{(k)}} \qquad \ell = 0, 1, \ldots$$

$$k = -\lfloor \tfrac{\ell+2}{2} \rfloor, -\lfloor \tfrac{\ell+2}{2} \rfloor + 1, \ldots$$

satisfying the conditions described in section 6 of part I.

(e) Chisholm's Padé approximants [CHISc]

$$R(x,y) = \frac{\sum_{i=0}^{n} \sum_{j=0}^{n} a_{ij} x^i y^j}{\sum_{i=0}^{n} \sum_{j=0}^{n} b_{ij} x^i y^j}$$

where a_{ij} and b_{ij} are computed so that in the Taylor series development

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

we have

$$c_{ij} = 0 \qquad (i,j) \in \{(i,j) \mid 0 \le i+j \le 2n\}$$

$$c_{2n+1-j,j} + c_{j,2n+1-j} = 0 \qquad j = 1, \ldots, 2n$$

(f) Levin's general order Padé approximants [LEVIa]

$$R(x,y) = \frac{\sum\limits_{(i,j)\in N} a_{ij}x^i y^j}{\sum\limits_{(i,j)\in D} b_{ij}x^i y^j}$$

described in full detail in section 6 of part I and satisfying

$$(f - R)(x,y) = \sum_{(i,j)\in \mathbb{N}^2\setminus I} c_{ij}x^i y^j$$

Our choice for the sets N, D and I is:

$$N = \{(i,j) \mid 0 \le i+j \le n_1\} \cup \{(\lfloor\frac{n_1+1}{2}\rfloor, \lfloor\frac{n_1+1}{2}\rfloor)\}$$

$$D = \{(i,j) \mid 0 \le i+j \le n_2\}$$

$$I = \{(i,j) \mid 0 \le i \le n_3, 0 \le j \le n_3\}$$

(g) General order rational interpolants

$$R(x,y) = \frac{\sum\limits_{(i,j)\in N} a_{ij}B_{ij}(x,y)}{\sum\limits_{(i,j)\in D} b_{ij}B_{ij}(x,y)}$$

as given by (I.3.5) here and with the next choice for the index sets N, D and I:

$$N = \{(i,j) \mid 0 \le i+j \le n_1\} \cup \{(\lfloor\frac{n_1+1}{2}\rfloor, \lfloor\frac{n_1+1}{2}\rfloor)\}$$

$$D = \{(i,j) \mid 0 \le i+j \le n_2\}$$

$$I = \{(i,j) \mid 0 \le i \le n_3, 0 \le j \le n_3\}$$

In order to use the same amount of data for each method, we are going to take

(a) $n_1 = 5$ and $n_2 = 5$
(b) $n = 5$ and $n_{ix} = 5 = n_{iy}$ $\quad i = 0, \ldots, 5$
(c) $n = 5$ and $n_i = 5$ $\quad i = 0, \ldots, 5$
(d) $n = 4$ and $m = 3$
(e) $n = 3$
(f) $n_1 = 5$, $n_2 = 4$ and $n_3 = 5$
(g) $\tilde{n}_1 = 5$, $\tilde{n}_2 = 4$ and $\tilde{n}_3 = 5$
For (a), (b), (c) and (g) the interpolation points are chosen to be

$$\begin{array}{lll} x_0 = 0.90 & x_1 = -0.85 & x_2 = 0.47 \\ x_3 = -0.54 & x_4 = 0.18 & x_5 = -0.23 \\ y_0 = 0.70 & y_1 = -0.77 & y_2 = 0.60 \\ y_3 = -0.45 & y_4 = 0.21 & y_5 = -0.35 \end{array}$$

which amounts to 36 data points (x_i, y_j). For (d), (e) and (f) respectively 36, 34 and 36 Taylor coefficients are given in order to compute the approximant, namely

$$\text{for (d): } \frac{\partial^{i+j} f}{\partial x^i \partial y^j}\Big|_{(1,1)} \qquad (i,j) \in \{(i,j) \mid 0 \le i+j \le 7\}$$

$$\text{for (e): } \frac{\partial^{i+j} f}{\partial x^i \partial y^j}\Big|_{(1,1)} \qquad (i,j) \in \{(i,j) \mid 0 \le i+j \le 6\} \cup \{(1,6),(2,5),\ldots,(5,2),(6,1)\}$$

$$\text{for (f): } \frac{\partial^{i+j} f}{\partial x^i \partial y^j}\Big|_{(1,1)} \qquad (i,j) \in \{(i,j) \mid 0 \le i \le 5 \, , 0 \le j \le 5\}$$

We take

$$(u_i, v_j) \in \{(-0.75, -0.75), (-0.50, -0.50), (-0.25, -0.25)\} \cup \{(0.25, 0.25), (0.50, 0.50), (0.75, 0.75)\}$$

The rational interpolants in (b) and (c) are computed using a backward evaluation algorithm while the rational interpolants from (g) are computed once using the algorithm given in (I.4.2) (see results (g)) and once using (I.5.4–7) (see results (g')). For the Padé approximants in (d) the well-known ε-algorithm is used while the Padé approximans from (e) and (f) are calculated once using (I.4.2) for the representation (I.6.4) (see results (e) and (f)) and once using the qdg-algorithm for the starting values (I.6.6) (see results (e') and (f')). Of course one can also compute the approximants in (e) and (f) by means of older techniques used by the Chisholm-group [GRAVa] and Levin themselves [LEVIb]. The numerical results can be found in table II.1.1 below. All the computations were performed in floating point double precision arithmetic on a Gould UTX/32 with an input of 12 significant decimal digits.

For all the types of approximants, except (c), the choice for $R(x, y)$ was such that it was a symmetric function. This was done because $B(x, y)$ is symmetric. We noticed that unsymmetric approximants yield worse numerical results. The polynomial approximants loose a number of significant digits because of the singularities of the Beta function. The ε-algorithm (d) and the other Padé approximants (e) and (f) get all their information at $(1, 1)$, far from the points (u_i, v_j). What's more, the given Taylor series does not even converge for $-1 < x, y < 0$. This is a disadvantage in comparison with the interpolation methods. As a conclusion we can say that the general order rational interpolants (g) introduced here, behave quite well.

	(−0.75, −0.75)	(−0.50, −0.50)	(−0.25, −0.25)
(a)	11.	0.06	−6.75
(b)	9.95	−0.001	−6.7770
(c)	9.95	0.003	−6.775
(d)	8.8	−0.07	−6.786
(e)	7.0	−0.14	−6.787
(e')	6.9	−0.14	−6.785
(f)	5.3	−0.46	−6.84
(f')	5.6	−0.41	−6.83
(g)	9.91	0.0002	−6.7776
(g')	9.91	−0.0002	−6.7776
B(x,y)	9.88839829	0.	−6.77770467

	(0.25, 0.25)	(0.50, 0.50)	(0.75, 0.75)
(a)	7.45	3.14151	1.69
(b)	7.416291	3.14159276	1.694426
(c)	7.416295	3.14159290	1.694426
(d)	7.416307	3.14159269	1.69442617
(e)	7.416310	3.14159269	1.69442617
(e')	7.4160	3.1416	1.69442617
(f)	7.4164	3.1415938	1.69442617
(f')	7.4164	3.1415936	1.69442617
(g)	7.416310	3.14159292	1.694426
(g')	7.416309	3.14159290	1.694426
B(x,y)	7.41629871	3.14159265	1.69442616

Table II.1.1

2. MULTIDIMENSIONAL CONVERGENCE ACCELERATION.

The idea of using the epsilon-algorithm to accelerate the convergence of a sequence, which can be considered as a table with single entry, is quite well-known. Given the sequence $\{a_i\}_{i \in \mathbb{N}}$ with $A = \lim_{i \to \infty} a_i$, we choose n and m in $\mathbb{N}$ and construct the ratio of determinants

$$\frac{\begin{vmatrix} a_n & a_{n-1} & \cdots & a_{n-m} \\ \nabla a_{n+1} & \nabla a_n & \cdots & \nabla a_{n+1-m} \\ \vdots & \vdots & \ddots & \vdots \\ \nabla a_{n+m} & \nabla a_{n+m-1} & \cdots & \nabla a_n \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & & 1 \\ \nabla a_{n+1} & \nabla a_n & \cdots & \nabla a_{n+1-m} \\ \vdots & \vdots & \ddots & \vdots \\ \nabla a_{n+m} & \nabla a_{n+m-1} & \cdots & \nabla a_n \end{vmatrix}} \qquad (II.2.1)$$

with $\nabla a_i = a_i - a_{i-1}$ and $a_i = 0$ for $i < 0$. The ratio (II.2.1) is the Padé approximant of order (n, m) evaluated at $x = 1$ for the univariate function

$$f(x) = \sum_{i=0}^{\infty} \nabla a_i x^i$$

We are particularly interested in approximations at $x = 1$ since

$$f(1) = A$$

This ratio of determinants can easily be computed using the epsilon-algorithm. With

$$\varepsilon_{-1}^{(k)} = 0 \qquad k = 0, 1, \ldots$$

$$\varepsilon_{0}^{(k)} = a_k \qquad k = 0, 1, \ldots$$

$$\varepsilon_{k+1}^{(\ell)} = \varepsilon_{k-1}^{(\ell+1)} + \frac{1}{\varepsilon_k^{(\ell+1)} - \varepsilon_k^{(\ell)}} \qquad k = 0, 1, \ldots \qquad \ell = 0, 1, \ldots$$

formula (II.2.1) is given by $\varepsilon_{2m}^{(n-m)}$. The ε-values are usually arranged in a table as follows

$$\begin{array}{ccccc}
\varepsilon_{-1}^{(0)} & & & & \\
 & \varepsilon_{0}^{(0)} & & & \\
\varepsilon_{-1}^{(1)} & & \varepsilon_{1}^{(0)} & & \\
 & \varepsilon_{0}^{(1)} & & \varepsilon_{2}^{(0)} & \\
\varepsilon_{-1}^{(2)} & & \varepsilon_{1}^{(1)} & & \ddots \\
\vdots & \varepsilon_{0}^{(2)} & \vdots & \varepsilon_{2}^{(1)} & \\
 & \vdots & & \vdots & \ddots
\end{array}$$

The epsilon-algorithm is called a **convergence accelerator** because it can be shown, in some cases, that the convergence of the columns or diagonals in the ε-table is faster than that of the given sequence $\{a_i\}_{i\in\mathbb{N}}$ [BREZa, pp. 83–85].

The previous reasoning was generalized by Brezinski. Given sequences $\{g_k(i)\}_{i\in\mathbb{N}}$ $(k = 1,2,\ldots)$ and $\{a_i\}_{i\in\mathbb{N}}$ with $A = \lim_{i\to\infty} a_i$ where approximately

$$a_i = A + \alpha_1 g_1(i) + \ldots + \alpha_m g_m(i) \qquad i \geq 0$$

it is easy to see that an approximate value for A is given by

$$\frac{\begin{vmatrix} a_n & a_{n-1} & \ldots & a_{n-m} \\ g_1(n) & \ldots & & g_1(n-m) \\ \vdots & & & \vdots \\ g_m(n) & & \ldots & g_m(n-m) \end{vmatrix}}{\begin{vmatrix} 1 & \ldots & & 1 \\ g_1(n) & \ldots & & g_1(n-m) \\ \vdots & & & \vdots \\ g_m(n) & & \ldots & g_m(n-m) \end{vmatrix}} \qquad (II.2.2)$$

In [BREZb] it is shown that formula (II.2.2) can be computed recursively in an analogous way as formula (II.2.1), now using the E-algorithm. With

$$E_0^{(k)} = a_k \qquad k = 0, 1, \ldots$$

$$g_{0,k}^{(\ell)} = g_k(\ell) \qquad k = 1, 2, \ldots \qquad \ell = 0, 1, \ldots$$

$$E_{k+1}^{(\ell)} = \frac{E_k^{(\ell)} g_{k,k+1}^{(\ell+1)} - E_k^{(\ell+1)} g_{k,k+1}^{(\ell)}}{g_{k,k+1}^{(\ell+1)} - g_{k,k+1}^{(\ell)}} \qquad \ell = 0, 1, \ldots \qquad k = 0, 1 \ldots$$

$$g_{k+1,j}^{(\ell)} = \frac{g_{k,j}^{(\ell)} g_{k,k+1}^{(\ell+1)} - g_{k,j}^{(\ell+1)} g_{k,k+1}^{(\ell)}}{g_{k,k+1}^{(\ell+1)} - g_{k,k+1}^{(\ell)}} \qquad j = k+1, k+2, \ldots$$

formula (II.2.2) is given by $E_m^{(n-m)}$. The values $E_{k+1}^{(\ell)}$ and $g_{k+1,j}^{(\ell)}$ are stored as in the tables I.4.1 and I.4.2 of part I. Convergence acceleration results are given in [BREZb]. So far for the univariate case.

Suppose we are given a table $\{a_{i_1 \ldots i_p}\}_{(i_1, \ldots, i_p) \in \mathbb{N}^p}$ with multiple entry and with $A = \lim_{i_1, \ldots, i_p \to \infty} a_{i_1 \ldots i_p}$. In [CUYTa] formula (II.2.1) is generalized for this case as follows. Define

$$f(x_1, \ldots, x_p) = \sum_{i_1, \ldots, i_p = 0}^{\infty} \nabla a_{i_1 \ldots i_p} x_1^{i_1} \ldots x_p^{i_p} \qquad (II.2.3a)$$

with

$$\begin{aligned} \nabla a_{i_1 \ldots i_p} = a_{i_1 \ldots i_p} &- \sum_{j=1}^{p} a_{i_1 \ldots (i_j - 1) \ldots i_p} \\ &+ \sum_{\substack{j,k=1 \\ j<k}}^{p} a_{i_1 \ldots i_{j-1} (i_j - 1) i_{j+1} \ldots i_{k-1} (i_k - 1) i_{k+1} \ldots i_p} \\ &- \ldots + (-1)^p a_{(i_1 - 1) \ldots (i_p - 1)} \end{aligned} \qquad (II.2.3b)$$

Clearly

$$f(1, \ldots, 1) = A$$

For this multivariate function multivariate Padé approximants can be calculated and evaluated at $(x_1, \ldots, x_p) = (1, \ldots, 1)$ via the epsilon-algorithm [CUYTa]. Let us restrict ourselves again to the bivariate case and deal with a table $\{a_{ij}\}_{(i,j)\in \mathbb{N}}$ of double entry. The bivariate Padé approximant of order (n, m) to which the epsilon-algorithm applies, is then given by

$$\frac{\begin{vmatrix} \sum_{i+j=0}^{n} \nabla a_{ij} & \cdots & \sum_{i+j=0}^{n-m} \nabla a_{ij} \\ \sum_{i+j=n+1} \nabla a_{ij} & \cdots & \sum_{i+j=n+1-m} \nabla a_{ij} \\ \vdots & & \vdots \\ \sum_{i+j=n+m} \nabla a_{ij} & \cdots & \sum_{i+j=n} \nabla a_{ij} \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ \sum_{i+j=n+1} \nabla a_{ij} & \cdots & \sum_{i+j=n+1-m} \nabla a_{ij} \\ \vdots & & \vdots \\ \sum_{i+j=n+m} \nabla a_{ij} & \cdots & \sum_{i+j=n} \nabla a_{ij} \end{vmatrix}} \tag{II.2.4}$$

where $\sum_{i+j=0}^{k} \nabla a_{ij}$ can be simplified to $\sum_{i+j=k} a_{ij} - \sum_{i+j=k-1} a_{ij}$. For convergence acceleration results we refer to [CUYTa].

The technique described above used the epsilon-algorithm for the evaluation of its Padé approximant. We discussed another recursive computation scheme for different definitions of multivariate Padé approximants in section 6 of part I which was based on the E-algorithm. In this way a number of multivariate convergence accelerators suggested in the past appear to be particular applications of the E-algorithm given above. Consider for instance the following transformation based on suggestions by Levin [LEVIb] and Albertsen, Jacobsen and Sørensen [ALBE]

$$\frac{\begin{vmatrix} a_{i_n-d_0,j_n-e_0} & \cdots & a_{i_n-d_m,j_n-e_m} \\ \nabla_0\, a_{i_{n+1}-d_0,j_{n+1}-e_0} & \cdots & \nabla_m\, a_{i_{n+1}-d_m,j_{n+1}-e_m} \\ \vdots & & \vdots \\ \nabla_0\, a_{i_{n+m}-d_0,j_{n+m}-e_0} & \cdots & \nabla_m\, a_{i_{n+m}-d_m,j_{n+m}-e_m} \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ \nabla_0\, a_{i_{n+1}-d_0,j_{n+1}-e_0} & \cdots & \nabla_m\, a_{i_{n+1}-d_m,j_{n+1}-e_m} \\ \vdots & & \vdots \\ \nabla_0\, a_{i_{n+m}-d_0,j_{n+m}-e_0} & \cdots & \nabla_m\, a_{i_{n+m}-d_m,j_{n+m}-e_m} \end{vmatrix}} \qquad (II.2.5)$$

where $\nabla_k a_{i_h-d_k,j_h-e_k} = a_{i_h-d_k,j_h-e_k} - a_{i_{h-1}-d_k,j_{h-1}-e_k}$. That this expression can be computed by means of the E-algorithm can easily be seen from the fact that it is a multivariate Padé aproximant of the type given in (I.6.4) for the function

$$f(x,y) = \sum_{h=0}^{\infty} \nabla a_{i_h j_h} x^{i_h} y^{j_h} \qquad (II.2.6)$$

where $\nabla a_{i_h j_h} = a_{i_h j_h} - a_{i_{h-1} j_{h-1}}$ and $a_{ij} = 0$ if $i < 0$ or $j < 0$. Remember that $(i_0, j_0), (i_1, j_1), (i_2, j_2), \ldots$ is a numbering in $I\!N^2$. The partial sums $t_0(\ell)$ and $t_r(\ell)$ necessary to start the E-algorithm are given by

$$\begin{aligned} t_0(\ell) &= \sum_{(i_h,j_h)\in N_\ell} \nabla a_{i_h j_h} x^{i_h} y^{j_h} \\ &= \sum_{h=0}^{\ell} \nabla a_{i_h j_h} x^{i_h} y^{j_h} \\ &= a_{i_\ell j_\ell} x^{i_\ell} y^{j_\ell} \end{aligned}$$

and

$$\begin{aligned} t_r(\ell) &= \sum_{(i_h,j_h)\in N_\ell} \nabla_r a_{i_h-d_r,j_h-e_r} x^{i_h-d_r} y^{j_h-e_r} \\ &= \sum_{h=0}^{\ell} \nabla_r a_{i_h-d_r j_h-e_r} x^{i_h-d_r} y^{j_h-e_r} \\ &= a_{i_\ell-d_r j_\ell-e_r} x^{i_\ell-d_r} y^{j_\ell-e_r} \end{aligned}$$

When Levin and Albertsen, Jacobsen and Sørensen developed their convergence accelerator, they did not know that recursive computation was possible and they computed formulas analogous to (II.2.5) by solving systems of linear equations.

Other formulas than (II.2.5) can be obtained by constructing multivariate general order Padé approximants for the series (II.2.3) instead of the series (II.2.6). An even more general formula than (II.2.5) is the one that results if we construct multivariate rational interpolants instead of multivariate Padé approximants. We refer the reader to the following section.

3. Some new convergence accelerators.

Let us first discuss new methods that result from the use of multivariate general order Padé approximants. Consider a two-dimensional table $\{a_{ij}\}_{(i,j)\in\mathbb{N}^2}$ with $\lim_{i,j\to\infty} a_{ij} = A$ and construct the series (II.2.3) with $f(1,1) = A$. If we choose a numbering in $\mathbb{N}^2$ and construct a sequence of sets $\{I_\ell\}_{\ell\in\mathbb{N}}$ with $\#I_\ell = \ell$, then for each $\ell = 0, 1, \ldots$ a variety of numerator and denominator index sets N_n and D_m with $n + m = \ell$ exists. The general order Padé approximants

$$[N_n/D_m]_{I_\ell}(1,1) \qquad (II.3.1)$$

for (II.2.3) can be computed by means of the E-algorithm and found in $E_m^{(n)}$.

In order to illustrate this technique numerically we consider the following situation. Suppose one wants to calculate the integral of a function $g(x, y)$ on a bounded closed domain Ω of $\mathbb{R}^2$. For the sake of simplicity we take $\Omega = [0,1] \times [0,1]$. The table $\{a_{ij}\}_{(i,j)\in\mathbb{N}^2}$ can for instance be obtained by subdividing the interval [0,1] in each direction respectively into 2^i and 2^j intervals of equal length $h_1 = 2^{-i}$ and $h_2 = 2^{-j}$. Using the midpoint rule one can then substitute approximations

$$\int_0^{h_1}\int_0^{h_2} g(x,y)\,dx\,dy = h_1 h_2 g(\frac{h_1}{2}, \frac{h_2}{2})$$

to calculate

$$a_{ij} = \frac{1}{2^{i+j}}\left(\sum_{k=1}^{2^i}\sum_{\ell=1}^{2^j} g\left(\frac{2k-1}{2^{i+1}}, \frac{2\ell-1}{2^{j+1}}\right)\right)$$

Let us take the diagonal enumeration of $\mathbb{N}^2$ given by (0,0), (1,0), (0,1), (2,0), (1,1), (0,2), ... As an example we take $g(x, y) = 1/(x + y)$ which produces slowly converging a_{ij} because of the singularity of the integrand in (0,0). Let the values a_{ij} be given for $0 \le i + j \le 9$. With these data the approximations (II.2.4), (II.2.5) and (II.3.1) can be computed respectively for $n + m = 0, \ldots, 9$ and $n + m = 0, \ldots, 54$ because (II.2.4) adds a complete diagonal of data in one step and (II.2.5) and (II.3.1) add the data along a diagonal one by one. The results displayed in table II.3.1 are the most accurate among the possible approximations $\varepsilon_{2m}^{(n-m)}$ and $E_m^{(n)}$ respectively for $n+m=i$ and $n+m+1=(i+1)(i+2)/2$ where $i \leq 9$. We can compare them with the $a_{\lfloor \frac{i+1}{2} \rfloor, \lfloor \frac{i}{2} \rfloor}$. The exact value of the integral is

$$\int_0^1 \int_0^1 \frac{1}{x+y}\, dx\, dy = 2 \ln 2 = 1.38629436\ldots$$

It is clear that (II.2.5) can be improved by (II.3.1). Similar conclusions can be found in the sequel of this section.

Table II.3.1

$a_{\lfloor \frac{i+1}{2} \rfloor, \lfloor \frac{i}{2} \rfloor}$	$\varepsilon_{2\lfloor \frac{i}{2} \rfloor}^{\lfloor \frac{i+1}{2} \rfloor - \lfloor \frac{i}{2} \rfloor}$	$(II.2.5)$	$(II.3.1)$
$a_{11} = 1.166667$	$\varepsilon_2^{(0)} = 1.330295$	$E_2^{(3)} = 1.292352$	$E_2^{(3)} = 1.183518$
$a_{21} = 1.209102$	$\varepsilon_2^{(1)} = 1.361764$	$E_3^{(6)} = 1.374224$	$E_3^{(6)} = 1.228489$
$a_{22} = 1.269048$	$\varepsilon_4^{(0)} = 1.396396$	$E_5^{(9)} = 1.359011$	$E_5^{(9)} = 1.304007$
$a_{32} = 1.292978$	$\varepsilon_4^{(1)} = 1.386057$	$E_8^{(12)} = 1.373649$	$E_8^{(12)} = 1.329994$
$a_{33} = 1.325744$	$\varepsilon_6^{(0)} = 1.386872$	$E_{10}^{(17)} = 1.385863$	$E_{10}^{(17)} = 1.360150$
$a_{43} = 1.338426$	$\varepsilon_6^{(1)} = 1.386481$	$E_{15}^{(20)} = 1.386177$	$E_{15}^{(20)} = 1.374274$
$a_{44} = 1.355532$	$\varepsilon_8^{(0)} = 1.386309$	$E_{18}^{(26)} = 1.386366$	$E_{18}^{(26)} = 1.371675$
$a_{54} = 1.362056$	$\varepsilon_8^{(1)} = 1.386298$	$E_{25}^{(29)} = 1.386298$	$E_{25}^{(29)} = 1.385897$

Secondly we shall discuss a technique that results from the use of multivariate general order rational interpolants. Consider a two-dimensional table $\{a_{ij}\}_{(i,j)\in \mathbb{N}^2}$ with $\lim_{i,j\to\infty} a_{ij} = A$ and let $\{(x_i, y_j)\}_{(i,j)\in \mathbb{N}^2}$ be a convergent table of points in $\mathbb{R}^2$ with

$$\lim_{i,j\to\infty} (x_i, y_j) = (z_1, z_2)$$

When using extrapolation techniques to accelerate the convergence of $\{a_{ij}\}_{(i,j)\in \mathbb{N}^2}$, we compute a sequence $\{b_i\}_{i\in \mathbb{N}}$ with

$$b_i = \lim_{(x,y)\to(z_1,z_2)} g_i(x,y)$$

where $g_i(x, y)$ is determined by some interpolation conditions. The point (z_1, z_2) is called the **extrapolation point.** In analogy with the univariate extrapolation technique of Bulirsch-Stoer, we choose for $g_i(x, y)$ the bivariate rational interpolants on the descending staircase

$$\begin{array}{lll} [N_0/D_0]_{I_0} & & \\ [N_1/D_0]_{I_1} & [N_1/D_1]_{I_2} & \\ & [N_2/D_1]_{I_3} & [N_2/D_2]_{I_4} \\ & \vdots & \quad \ldots \end{array} \qquad (I.5.1)$$

For the notation we refer to the sections 3 and 5 of part I. These rational interpolants

$$[N_n/D_m]_{I_{n+m}} = \frac{p_n(x, y)}{q_m(x, y)}$$

are constructed here such that

$$a_{ij} = \frac{p_n(x_i, y_j)}{q_m(x_i, y_j)} \qquad (i, j) \in I_{n+m} \subseteq I\!N^2$$

and then b_i is computed from

$$b_i = \frac{p_n(z_1, z_2)}{q_m(z_1, z_2)} \qquad n = s + \lfloor \tfrac{i+1}{2} \rfloor \qquad m = \lfloor \tfrac{i}{2} \rfloor \qquad i = 0, 1, 2 \ldots \qquad (II.3.2)$$

Of course the choice of the interpolation points (x_i, y_j) greatly influences the convergence behaviour of the resulting sequence $\{b_i\}_{i \in I\!N}$.

Let us compare the formulas (II.2.5), (II.3.1) and (II.3.2) numerically. We know that the Beta function $B(x, y)$ for $-1 < x, y < 0$ can be written as

$$B(x, y) = \frac{1 + xyw(x + 1, y + 1)}{xy(x + 1)(y + 1)} (x + y)(1 + x + y)$$

and that a Taylor series development for $w(x + 1, y + 1)$ can be computed by the first method suggested in [GRAVa]. Let us denote this Taylor series by

$$w(x + 1, y + 1) = \sum_{i,j=0}^{\infty} c_{0i,0j} x^i y^j$$

and its partial sums for $(x,y)=(u,v)$ by

$$a_{k\ell} = \sum_{i=0}^{k} \sum_{j=0}^{\ell} c_{0i,0j} u^i v^j$$

Input of the convergence accelerators are these bivariate partial sums of the Taylor series development for $w(x+1,y+1)$ around $(1,1)$. We shall compute rational approximants and interpolants $R(u,v)$ for $w(u+1,v+1)$ and compare the value

$$\frac{1+uvR(u,v)}{uv(u+1)(v+1)}(u+v)(1+u+v)$$

with $B(u,v)$. Let the values $a_{k\ell}$ be given for $(k,\ell) \in I \subseteq \mathbb{N}^2$. Let us associate each $a_{k\ell}$ with an interpolation point (x_k, y_ℓ) where

$$\lim_{k,\ell\to\infty} (x_k, y_\ell) = (z_1, z_2)$$

$$\lim_{k,\ell\to\infty} a_{k\ell} = w(u,v)$$

So we construct a function $f(x,y)$ satisfying

$$f(x_k, y_\ell) = a_{k\ell}$$

$$f(z_1, z_2) = w(u,v)$$

We can then proceed as in the sections 3 and 4, choosing numerator and denominator index sets N and D, constructing subsets N_ℓ, D_ℓ and I_ℓ, computing rational interpolants $[N_n/D_m]_{I_{n+m}}$ for $f(x,y)$ and evaluating them at (z_1,z_2). In our example we have taken $(u,v)=(-0.92,-0.97)$. In the first column the values

$$\frac{1+uv\,a_{ii}}{uv(u+1)(v+1)}(u+v)(1+u+v)$$

are displayed. For the construction of all the other columns we have taken

$$I = \{(k,\ell) \mid 0 \le k,\ell \le 6\}$$

and used the enumeration (0,0), (1,0), (0,1), (1,1), (2,0), (0,2), (2,1), (1,2), (2,2), (3,0), (0,3), (3,1), (1,3), (3,2), (2,3), (3,3), ... In order to compare values that use the same number of data as the a_{ii} for $i = 0, 1, 2, \ldots$, we choose for $R(x, y)$ the $(i+1)^{2\,th}$ elements on the descending staircase given at the beginning of this section, namely

$$\begin{array}{ll} i = 0: & [N_0/D_0]_{I_0} \\ i = 1: & [N_2/D_1]_{I_3} \\ i = 2: & [N_4/D_4]_{I_8} \\ i = 3: & [N_8/D_7]_{I_{15}} \\ i = 4: & [N_{12}/D_{12}]_{I_{24}} \\ i = 5: & [N_{18}/D_{17}]_{I_{35}} \end{array}$$

The second column is an illustration of (II.2.5) and the third column an illustration of (II.3.1). The other columns illustrate (II.3.2) where we have made different choices for the interpolation points:

$$(x_k, y_\ell) = (\frac{1}{k+1}, \frac{1}{\ell+1}) \qquad (II.3.2a)$$

$$(x_k, y_\ell) = (2^{-k}, 2^{-\ell}) \qquad (II.3.2b)$$

The correct limit is

$$A = B(-0.92, -0.97) = 86.07672\ldots$$

All computations are performed on a Gould UTX/32 in double precision arithmetic. Remark that the values a_{ii} converge slowly due to the presence of singularities in the vicinity of $(u, v) = (-0.92, -0.97)$. For similar conclusions we refer to section 1 of part II. Our advice to the reader is to consider construction of the series (II.2.3) if Padé approximants are used and to pay attention to the choice of the interpolation points if rational interpolants are used.

Table II.3.2

i	a_{ii}	$(II.2.5)$	$(II.3.1)$	$(II.3.2a)$	$(II.3.2b)$
1	118.551	106.835	140.066	23.0915	23.0915
2	92.1841	88.6788	83.1745	100.396	88.2749
3	88.3833	87.6991	86.8761	78.0438	85.7630
4	87.1083	73.6345	86.1894	86.5946	86.0138
5	86.5533	93.2420	86.0873	83.8083	86.0543
6	86.3002	85.8025	86.0793	86.8151	86.0689

Several theorems exist that describe the type of series which can be summed exactly by a particular convergence accelerator in that sense that an application of the convergence accelerator to the sequence of its partial sums gives the limit value A. Consider for instance formula (II.2.1) again. According to [BREZa, pp.40–42] a necessary and sufficient condition for

$$\varepsilon_{2m}^{(n-m)} = A \qquad n-m = \ell, \ell+1, \ldots$$

is that there exist constants $\alpha_0, \ldots, \alpha_m$ with $\sum_{k=0}^{m} \alpha_k \neq 0$, such that

$$\sum_{k=0}^{m} \alpha_k (a_{n-m+k} - A) = 0 \qquad n-m = \ell, \ell+1, \ldots \qquad (II.3.2)$$

This can easily be seen by solving (II.3.2) using Cramer's rule.

When using (II.2.2) instead of (II.2.1), formula (II.3.2) generalizes as follows. A necessary and sufficient condition for the exact summation [BREZb]

$$E_m^{(n-m)} = A \qquad n-m = \ell, \ell+1, \ldots$$

is

$$a_{n-m} = A + \sum_{k=1}^{m} \alpha_k g_k(n-m) \qquad n-m = \ell, \ell+1, \ldots \qquad (II.3.3)$$

When turning to the multivariate case analogous conclusions can be written down. The summation process (II.2.4) sums the series

$$\sum_{i,j=0}^{\infty} \nabla a_{ij}$$

exactly, if

$$\sum_{k=0}^{m} \alpha_k \left(\sum_{i+j=0}^{n-m+k} \nabla a_{ij} - A \right) = 0 \qquad (II.3.4)$$

with $\sum_{k=0}^{m} \alpha_k \neq 0$.

An even more general result was proved by [BREZc] for (II.2.5). When computed recursively as suggested in section 4 of part I, the expression (I.2.4) is given by $E_m^{(n)}$. A necessary and sufficient condition for exact summation of

$$\sum_{h=0}^{\infty} \nabla a_{i_h j_h} \qquad (II.3.5)$$

is that there exist $\alpha_0, \ldots, \alpha_m$ not all zero such that

$$\sum_{k=0}^{m} \alpha_k (a_{i_n - d_k, j_n - e_k} - A) = 0$$

We have not mentioned the most general results here because this would take away much of the clarity when we try to show how things generalize. The reader can now translate more general conditions than (II.3.2) and (II.3.3) to the multivariate case. We conclude with a necessary and sufficient condition for our new convergence accelerator to sum the series (II.3.5) exactly. It is a simple application of results given in [BREZc].

COROLLARY II.3.1. *A necessary and sufficient condition for exact summation of the series (II.3.5) by $[N_n/D_m]_{I_{n+m}} = p_n(x,y)/q_m(x,y)$ $(n \geq \ell)$, satisfying*

$$\frac{p_n}{q_m}(x_i, y_j) = a_{ij} \qquad (i,j) \in I_{n+m}$$

is that there exist $\alpha_0, \ldots, \alpha_m$ not all zero such that for $n \geq \ell$

$$\alpha_0(t_0(n) - A) + \ldots + \alpha_m(t_m(n) - A) = 0$$

where for $0 \leq k \leq m$

$$t_k(0) = c_{d_k i_0, e_k j_0} B_{d_k i_0, e_k j_0}(x, y)$$

$$t_k(n) = \sum_{(i,j)\in N_n} c_{d_k i, e_k j} B_{d_k i, e_k j}(x, y)$$

with

$$c_{d_k i, e_k j} = f[x_{d_k}, \dots, x_i][y_{e_k}, \dots, y_j]$$
$$f[x_i][y_j] = a_{ij}$$
$$c_{d_k i, e_k j} = 0 \qquad i < d_k \text{ or } j < e_k$$

4. NONLINEAR METHODS FOR THE SOLUTION OF SYSTEMS OF NONLINEAR EQUATIONS.

Suppose we want to find a root x^* of the nonlinear equation

$$f(x) = 0$$

Here the function f may be real- or complex-valued. If f is now replaced by a local approximation then a zero of that local approximation could be considered as an approximation for x^*. Methods based on this reasoning are called **direct**. One could also consider the inverse function g of f in a neighbourhood of the origin, if it exists, and replace g by a local approximation. Then an evaluation of this local approximation in 0 could be considered as an approximation for x^* since

$$g(0) = x^*$$

Methods using this technique are called **inverse**. Let us recapitulate the univariate situation.

Let x_i be an approximation for the root x^* of f and let

$$r_i(x) = \frac{p_i}{q_i}(x) \qquad (II.4.1a)$$

be the Padé approximant of order (n, m) for f in x_i. Then the next approximation x_{i+1} is calculated such that

$$p_i(x_{i+1}) = 0 \qquad (II.4.1b)$$

In case $p_i(x)$ is linear ($n = 1$) the value x_{i+1} is uniquely determined. It is clear that this is to be preferred for the sake of simplicity. A well-known method obtained in this way is Newton's method ($n = 1, m = 0$) which can be derived as follows. The Taylor series expansion for $f(x)$ at x_i is given by

$$f(x) = f(x_i) + f'(x_i)(x - x_i) + \frac{f''(x_i)}{2}(x - x_i)^2 + \dots \qquad (II.4.2)$$

Hence the Padé approximant of order $(1,0)$ for f at x_i equals

$$r_i(x) = f(x_i) + f'(x_i)(x - x_i)$$

and we obtain

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \qquad (II.4.3)$$

Another famous method is Halley's method based on the use of the Padé approximant of order $(1,1)$ for f at x_i:

$$x_{i+1} = x_i - \frac{f(x_i)/f'(x_i)}{1 - \frac{1}{2}f''(x_i)\frac{f(x_i)}{f'(x_i)^2}} \qquad (II.4.4)$$

Since the iterative procedures (II.4.3) and (II.4.4) only use information in the point x_i to calculate the next iterationpoint x_{i+1} they are called **one-point**. It is obvious that methods based on the use of (n,m) Padé approximants for f with $m > 0$ give better results if the function f has singularities.

The formulas (II.4.3) and (II.4.4) can also be generalized for the solution of a system of nonlinear equations

$$\begin{cases} f_1(x_1,\ldots,x_k) = 0 \\ \vdots \\ f_k(x_1,\ldots,x_k) = 0 \end{cases}$$

which we shall write as

$$F(x_1,\ldots,x_k) = 0$$

Newton's method can then be expressed as [ORTE]

$$\begin{pmatrix} x_1^{(i+1)} \\ \vdots \\ x_k^{(i+1)} \end{pmatrix} = \begin{pmatrix} x_1^{(i)} \\ \vdots \\ x_k^{(i)} \end{pmatrix} - F'(x_1^{(i)},\ldots,x_k^{(i)})^{-1} \begin{pmatrix} f_1(x_1^{(i)},\ldots,x_k^{(i)}) \\ \vdots \\ f_k(x_1^{(i)},\ldots,x_k^{(i)}) \end{pmatrix} \qquad (II.4.5)$$

where $F'(x_1^{(i)},\dots,x_k^{(i)})$ is the Jacobian matrix of first partial derivatives evaluated at $(x_1^{(i)},\dots,x_k^{(i)})$ with

$$F'(x_1,\dots,x_k) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_k} \\ \vdots & & \vdots \\ \frac{\partial f_k}{\partial x_1} & \cdots & \frac{\partial f_k}{\partial x_k} \end{pmatrix}$$

Let us now introduce the abbreviations

$$F_i = F(x_1^{(i)},\dots,x_k^{(i)})$$
$$F_i' = F'(x_1^{(i)},\dots,x_k^{(i)})$$

To generalize Halley's method we first rewrite (II.4.4) as

$$x_{i+1} = x_i + \frac{(-f(x_i)/f'(x_i))^2}{\frac{-f(x_i)}{f'(x_i)} + \frac{f''(x_i)f(x_i)^2}{2f'(x_i)^3}}$$

Then for the solution of a system of equations it becomes [CUYTi]

$$\begin{pmatrix} x_1^{(i+1)} \\ \vdots \\ x_k^{(i+1)} \end{pmatrix} = \begin{pmatrix} x_1^{(i)} \\ \vdots \\ x_k^{(i)} \end{pmatrix} +$$

$$+ \frac{(-F_i'^{-1}F_i)^2}{-F_i'^{-1}F_i + \frac{1}{2}F_i'^{-1}F''(x_1^{(i)},\dots,x_k^{(i)})[-F_i'^{-1}F_i, -F_i'^{-1}F_i]} \tag{II.4.6}$$

where the division and the square are performed componentwise and $F''(x_1,\dots,x_k)$ is the hypermatrix of second partial derivatives given by

$$F''(x_1,\dots,x_k) =$$

$$\begin{pmatrix} \frac{\partial^2 f_1}{\partial x_1^2} \cdots \frac{\partial^2 f_1}{\partial x_k \partial x_1} & \frac{\partial^2 f_1}{\partial x_1 \partial x_2} \cdots \frac{\partial^2 f_1}{\partial x_k \partial x_2} & \cdots & \frac{\partial^2 f_1}{\partial x_1 \partial x_k} \cdots \frac{\partial^2 f_1}{\partial x_k^2} \\ \vdots \quad\quad \vdots & \vdots \quad\quad \vdots & & \vdots \quad\quad \vdots \\ \frac{\partial^2 f_k}{\partial x_1^2} \cdots \frac{\partial^2 f_k}{\partial x_k \partial x_1} & \frac{\partial^2 f_k}{\partial x_1 \partial x_2} \cdots \frac{\partial^2 f_k}{\partial x_k \partial x_2} & \cdots & \frac{\partial^2 f_k}{\partial x_1 \partial x_k} \cdots \frac{\partial^2 f_k}{\partial x_k^2} \end{pmatrix}$$

which we have to multiply twice with the vector $-F_i'^{-1}F_i$. This multiplication is performed as follows. The hypermatrix $F''(x_1,\ldots,x_k)$ is a row of k matrices, each $k\times k$. If we use the usual matrix-vector multiplication for each element in the row we obtain

$$F''(x_1,\ldots,x_k)\begin{pmatrix} y_1\\ \vdots \\ y_k\end{pmatrix}\begin{pmatrix} y_1\\ \vdots \\ y_k\end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{k} \frac{\partial^2 f_1}{\partial x_1 \partial x_i} y_i & \cdots & \sum_{i=1}^{k} \frac{\partial^2 f_1}{\partial x_k \partial x_i} y_i \\ \vdots & & \vdots \\ \sum_{i=1}^{k} \frac{\partial^2 f_k}{\partial x_1 \partial x_i} y_i & \cdots & \sum_{i=1}^{k} \frac{\partial^2 f_k}{\partial x_k \partial x_i} y_i \end{pmatrix}\begin{pmatrix} y_1\\ \vdots \\ y_k\end{pmatrix}$$

In [CUYTi] is proved that the iterative procedure (II.4.6) actually results from the use of multivariate Padé approximants of order (1,1) for the inverse operator of $F(x_1,\ldots,x_k)$ at $(x_1^{(i)},\ldots,x_k^{(i)})$.

To illustrate the use of the formulas (II.4.5) and (II.4.6) we shall now solve the nonlinear system

$$\begin{cases} f_1(x,y) = e^{-x+y} - 0.1 = 0 \\ f_2(x,y) = e^{-x-y} - 0.1 = 0 \end{cases}$$

which has a simple root at

$$\begin{pmatrix} -\ln(0.1) \\ 0. \end{pmatrix} = \begin{pmatrix} 2.302585092994046 \\ 0. \end{pmatrix}$$

As initial point we take $(x^{(0)},y^{(0)}) = (4.3, 2.0)$. In the tables II.4.1 and II.4.2 one finds respectively the consecutive iterationsteps of Newton's and Halley's method. All computations are performed on a VAX 11–780 in double precision arithmetic. Halley's method behaves much better than the polynomial method of Newton because the inverse operator G of the system of equations F has a singularity near to the origin and this singularity causes trouble if we get close to it. For

$$F(x,y) = \begin{pmatrix} f_1(x,y) \\ f_2(x,y) \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix}$$

we can write

$$G(u,v) = \begin{pmatrix} g_1(u,v) \\ g_2(u,v) \end{pmatrix} = \begin{pmatrix} -0.5\,(\ln(0.1+u) + \ln(0.1+v)) \\ 0.5\,(\ln(0.1+u) - \ln(0.1+v)) \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}$$

With $(x^{(0)},y^{(0)}) = (4.3, 2.0)$ the value $v^{(0)} = f_2(x^{(0)},y^{(0)})$ is close to -0.1 which is close to the singularity of G.

Table II.4.1

i	$x^{(i)}$	$y^{(i)}$
0	$0.43000000D+01$	$0.20000000D+01$
1	$-0.22427305D+02$	$-0.24729886D+02$
2	$-0.21927303D+02$	$-0.24229888D+02$
3	$-0.21427303D+02$	$-0.23729888D+02$
4	$-0.20927303D+02$	$-0.23229888D+02$
5	$-0.20427303D+02$	$-0.22729888D+02$
6	$-0.19927303D+02$	$-0.22229888D+02$
7	$-0.19427303D+02$	$-0.21729888D+02$
8	$-0.18927303D+02$	$-0.21229888D+02$
9	$0.18427303D+02$	$-0.20729888D+02$
10	$-0.17927303D+02$	$-0.20229888D+02$
11	$-0.17427303D+02$	$-0.19729888D+02$
12	$-0.16927303D+02$	$-0.19229888D+02$
13	$-0.16427303D+02$	$-0.18729888D+02$
14	$-0.15927303D+02$	$-0.18229888D+02$
15	$-0.15427303D+02$	$-0.17729888D+02$
16	$-0.14927303D+02$	$-0.17229888D+02$
17	$-0.14427303D+02$	$-0.16729888D+02$
18	$-0.13927303D+02$	$-0.16229888D+02$
19	$-0.13427303D+02$	$-0.15729888D+02$
20	$-0.12927303D+02$	$-0.15229888D+02$

Table II.4.2

i	$x^{(i)}$	$y^{(i)}$
0	$0.43000000D+01$	$0.20000000D+01$
1	$0.28798400D+01$	$0.57957286D+00$
2	$0.22495475D+01$	$-0.52625816D-01$
3	$0.23018229D+01$	$-0.44901947D-02$
4	$0.23025841D+01$	$-0.57154737D-05$
5	$0.23025851D+01$	$-0.97689305D-11$
6	$0.23025851D+01$	$-0.17438130D-16$

The reasoning in (II.4.1) can be generalized by using rational interpolants instead of Padé approximants as local approximations for $f(x)$. Let

$$r_i(x) = \frac{p_i}{q_i}(x)$$

with p_i and q_i respectively of degree n and m, be such that in approximations $x_i, \ldots, x_{i-s}$ for the root x^* of f

$$\begin{aligned} r_i^{(j)}(x_i) &= f^{(j)}(x_i) \qquad j = 0, \ldots, \ell_0 - 1 \\ r_i^{(j)}(x_{i-1}) &= f^{(j)}(x_{i-1}) \qquad j = 0, \ldots, \ell_1 - 1 \\ &\vdots \\ r_i^{(j)}(x_{i-s}) &= f^{(j)}(x_{i-s}) \qquad j = 0, \ldots, \ell_s - 1 \end{aligned} \qquad (II.4.7a)$$

with $n+m+1 = \sum_{j=0}^{s} \ell_j$. Then the next iterationstep x_{i+1} is computed such that

$$p_i(x_{i+1}) = 0 \qquad (II.4.7b)$$

For the calculation of x_{i+1} we now use information in more than one previous point. Hence such methods are called **multipoint.**

If we restrict ourselves to the case $n = 1$, $m = 1$, $\ell = 1$ and $s = 2$. Then x_{i+1} is given by

$$x_{i+1} = x_i - \frac{f(x_i)[f(x_{i-1}) - f(x_{i-2})]}{f(x_{i-1})\dfrac{f(x_{i-2}) - f(x_i)}{x_{i-2} - x_i} - f(x_{i-2})\dfrac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}} \qquad (II.4.8)$$

Take $n = 1$, $m = 1$, $\ell_0 = 2$, $\ell_1 = 1$ and $s = 1$. Then x_{i+1} is given by

$$x_{i+1} = x_i + \frac{f(x_i)(x_i - x_{i-1})}{f(x_{i-1})f'(x_i)\dfrac{(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})} - f(x_i)} \qquad (II.4.9)$$

The case $n = 1$, $m = 0$, $\ell = 1$ and $s = 1$ reduces to the secant method.

By means of the multivariate rational Hermite interpolants introduced in part I, the previous formulas will now be generalized for the solution of systems of nonlinear equations.

5. METHODS BASED ON THE USE OF GENERAL ORDER RATIONAL INTERPOLANTS.

We use the same notations as in part I and as in the previous section. For each of the multivariate functions $f_j(x_1,\ldots,x_k)$ with $j=1,\ldots,k$ we choose

$$D = N = \{(0,\ldots,0),(1,0,\ldots,0),(0,1,0,\ldots,0),\ldots,(0,\ldots,0,1)\} \subset \mathbb{N}^k$$

$$H = \{(2,0,\ldots,0),(0,2,0,\ldots,0),\ldots,(0,\ldots,0,2)\} \subset \mathbb{N}^k$$

Here the interpolationset $N \cup H$ expresses interpolation conditions in the points

$$\left(x_1^{(i)},\ldots,x_k^{(i)}\right),\left(x_1^{(i-1)},x_2^{(i)},\ldots,x_k^{(i)}\right),\ldots,\left(x_1^{(i)},\ldots,x_{k-1}^{(i)},x_k^{(i-1)}\right),$$

$$\left(x_1^{(i-2)},x_2^{(i)},\ldots,x_k^{(i)}\right),\ldots,\left(x_1^{(i)},\ldots,x_{k-1}^{(i)},x_k^{(i-2)}\right)$$

Remark that this set of interpolation points is constructed from only three successive iteration points. The numerator of

$$r_{i_j}(x_1,\ldots,x_k) = \frac{p_{i_j}}{q_{i_j}}(x_1,\ldots,x_k) \qquad (II.5.1a)$$
$$= \frac{\sum_{(j_1,\ldots,j_k)\in N} a_{j_1\ldots j_k} B_{j_1\ldots j_k}(x_1,\ldots,x_k)}{\sum_{(j_1,\ldots,j_k)\in D} b_{j_1\ldots j_k} B_{j_1\ldots j_k}(x_1,\ldots,x_k)} \qquad j=1,\ldots,k$$

satisfying

$$(f_j q_{i_j} - p_{i_j})(x_1,\ldots,x_k) = \sum_{(\ell_1;\ldots;\ell_k)\in \mathbb{N}^k\setminus(N\cup H)} d_{\ell_1\ldots\ell_k} B_{\ell_1\ldots\ell_k}(x_1,\ldots,x_k)$$

where

$$B_{\ell_1\ldots\ell_k}(x_1,\ldots,x_k) = \prod_{\ell=0}^{\ell_1-1}(x_1 - x_1^{(i-\ell)})\ldots\prod_{\ell=0}^{\ell_k-1}(x_k - x_k^{(i-\ell)})$$

with possible coalescence of points, is then given by

$$p_{i_j}(x_1, \ldots, x_k) =$$

$$\begin{vmatrix} N_{0,\ldots,0}(x_1,\ldots,x_k) & N_{1,0,\ldots,0}(x_1,\ldots,x_k) & \ldots & N_{0,\ldots,0,1}(x_1,\ldots,x_k) \\ c_{02,00,\ldots,00} & c_{12,00,\ldots,00} & \ldots & 0 \\ \vdots & & \ddots & \\ c_{00,\ldots,00,02} & 0 & \ldots & c_{00,\ldots,00,12} \end{vmatrix}$$

where

$$N_{i_1,\ldots,i_k}(x_1,\ldots,x_k) = \sum_{(\ell_1,\ldots,\ell_k)\in N} c_{i_1\ell_1,\ldots,i_k\ell_k} B_{\ell_1\ldots\ell_k}(x_1,\ldots,x_k)$$

The values $c_{s_1t_1,\ldots,s_kt_k}$ are multivariate divided differences with possible coalescence of points. Remark that this formula is only valid if the set H provides a system of linearly independent equations. The next iterationstep $(x_1^{(i+1)}, \ldots, x_k^{(i+1)})$ is then constructed such that

$$\begin{cases} p_{i_1}(x_1^{(i+1)}, \ldots, x_k^{(i+1)}) = 0 \\ \vdots \\ p_{i_k}(x_1^{(i+1)}, \ldots, x_k^{(i+1)}) = 0 \end{cases} \qquad (II.5.1b)$$

For $k = 1$ and without coalescence of points this procedure coincides with the univariate iterative method (II.4.8). With $k = 2$ and without coalescence of points we obtain a bivariate generalization of (II.4.8). Let us use this technique to solve the system

$$\begin{cases} e^{-x+y} = 0.1 \\ e^{-x-y} = 0.1 \end{cases}$$

with initial points $(3.2, -0.95)$, $(3.4, -1.15)$ and $(3.3, -1.00)$. The numerical results computed in double precision are displayed in table II.5.1. The simple root is $(2.302585092994046, 0.)$.

It must be clear from part I that a whole variety of choices for the sets N, D and H is possible, depending on which multivariate divided differences can be computed. Some function evaluations may be much more difficult or time consuming than others. An advantage of iterative procedures that only use function evaluations is that no derivatives must be supplied although nowadays automatic differentiation takes away much of the laborious and erroneous work.

In the same way we can also derive a discretized Newton method in which the partial derivatives of the Jacobian matrix are approximated by difference quotients:

$$N = H = \{(0,\ldots,0),(1,0,\ldots,0),\ldots,(0,\ldots,0,1)\}$$
$$D = \{(0,\ldots,0)\}$$

$$\frac{\partial f_j}{\partial x_\ell}\Big|_{(x_1^{(i)},\ldots,x_k^{(i)})} \approx \frac{f_j(x_1^{(i)},\ldots,x_{\ell-1}^{(i)},x_\ell^{(i-1)},x_{\ell+1}^{(i)},\ldots,x_k^{(i)}) - f_j(x_1^{(i)},\ldots,x_k^{(i)})}{x_\ell^{(i-1)} - x_\ell^{(i)}}$$

If we call this matrix of difference quotients ΔF_i, then the next iterate is computed by means of

$$\begin{pmatrix} x_1^{(i+1)} \\ \vdots \\ x_k^{(i+1)} \end{pmatrix} = \begin{pmatrix} x_1^{(i)} \\ \vdots \\ x_k^{(i)} \end{pmatrix} - (\Delta F_i)^{-1} \begin{pmatrix} f_1(x_1^{(i)},\ldots,x_k^{(i)}) \\ \vdots \\ f_k(x_1^{(i)},\ldots,x_k^{(i)}) \end{pmatrix}$$

As an example we take the same system of equations and the same but fewer initial points as above. The consecutive iterationsteps computed in double precision can now be found in table II.5.2. The rational method is again giving better results. Now the initial points are such that $u = f_1(x,y)$ is close to -0.1 which is precisely a singularity of the inverse operator for the considered system of nonlinear equations.

Table II.5.1

i	$x^{(i)}$	$y^{(i)}$
	$0.32000000D+01$	$-0.95000000D+00$
	$0.34000000D+01$	$-0.11500000D+01$
0	$0.33000000D+01$	$-0.10000000D+01$
1	$0.25249070D+01$	$-0.22072875D+00$
2	$0.22618832D+01$	$0.41971944D-01$
3	$0.23127609D+01$	$-0.10164490D-01$
4	$0.23030978D+01$	$-0.51269373D-03$
5	$0.23025801D+01$	$0.49675854D-05$
6	$0.23025851D+01$	$-0.25696929D-08$
7	$0.23025851D+01$	$-0.12778916D-13$
8	$0.23025851D+01$	$-0.11350932D-16$

Table II.5.2

i	$x^{(i)}$	$y^{(i)}$
	$0.34000000D+01$	$-0.11500000D+01$
0	$0.33000000D+01$	$-0.10000000D+01$
1	$-0.29618530D+00$	$0.21743633D+01$
2	$0.32743183D+01$	$0.20884933D+01$
3	$0.22114211D+01$	$-0.84011352D+01$
4	$0.36513339D+01$	$-0.72149651D+01$
5	$-0.17900983D+04$	$0.20854111D+04$

Another system of nonlinear equations illustrates the possibilities of this newly developed technique. Consider [PÖNI]

$$\begin{cases} f_1(x, y) = x^2 - xy + y^2 + x - 2 = 0 \\ f_2(x, y) = 3x^2 + 2xy + 2y - 7 = 0 \end{cases}$$

which has a simple root in $(1, 1)$. This solution is also a bifurcation point because the Jacobian of the system of equations is singular. Therefore Newton-like methods are inappropriate because good approximations to the Jacobian will be ill-conditioned. The computation of bifurcation points is interesting because, from a physical point of view, they are points of unstable equilibrium. This implies that many methods require very accurate starting points. We solve the above system with much rougher starting values than in [PÖNI]. The results can be found in table II.5.3.

Table II.5.3

i	$x^{(i)}$	$y^{(i)}$
	$0.998000000D+00$	$1.00200000D+00$
	$0.996000000D+00$	$1.00300000D+00$
0	$0.997000000D+00$	$1.00400000D+00$
1	$0.998801518D+00$	$1.00239696D+00$
2	$0.999401241D+00$	$1.00119752D+00$
3	$0.999700529D+00$	$1.00059894D+00$
4	$0.999850224D+00$	$1.00029955D+00$
5	$0.999925102D+00$	$1.00014930D+00$
6	$0.999962549D+00$	$1.00007490D+00$
7	$0.999981274D+00$	$1.00003745D+00$
8	$0.999990637D+00$	$1.00001873D+00$
9	$0.999995318D+00$	$1.00000936D+00$
10	$0.999997659D+00$	$1.00000468D+00$
11	$0.999998830D+00$	$1.00000234D+00$
12	$0.999999415D+00$	$1.00000117D+00$
13	$0.999999707D+00$	$1.00000059D+00$
14	$0.999999854D+00$	$1.00000029D+00$
15	$0.999999927D+00$	$1.00000015D+00$
16	$0.999999964D+00$	$1.00000007D+00$
17	$0.999999982D+00$	$1.00000004D+00$
18	$0.999999991D+00$	$1.00000002D+00$
19	$0.999999996D+00$	$1.00000001D+00$
20	$0.999999999D+00$	$1.00000000D+00$

6. Methods based on the use of general order Padé approximants.

In section 4 we have generalized the iterative procedure (II.4.4) to the multivariate case by using the multivariate Padé approximants introduced in [CUYTf]. We have seen in section 6 of part I that these multivariate Padé approximants can be considered as multivariate general order Padé approximants. Let us first study this matter in more detail with respect to the iterative procedure (II.4.6) for the solution of

$$F(x) = F(x_1, \ldots, x_k) = \begin{pmatrix} f_1(x_1, \ldots, x_k) \\ \vdots \\ f_k(x_1, \ldots, x_k) \end{pmatrix} = 0$$

We denote the inverse of the Jacobian in $(x_1^{(i)}, \ldots, x_k^{(i)})$ by

$$F_i'^{-1} = L^{(i)} = \left(\ell_{rs}^{(i)}\right)_{r,s=1}^{k}$$

The series development for the inverse operator

$$G : \mathbb{R}^k \to \mathbb{R}^k : \begin{pmatrix} y_1 \\ \vdots \\ y_k \end{pmatrix} = \begin{pmatrix} f_1(x_1, \ldots, x_k) \\ \vdots \\ f_k(x_1, \ldots, x_k) \end{pmatrix} \to \begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix}$$

at $(y_1, \ldots, y_k) = F(x^{(i)})$ is given by

$$\begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix} = \begin{pmatrix} x_1^{(i)} \\ \vdots \\ x_k^{(i)} \end{pmatrix} + L^{(i)} \begin{pmatrix} f_1(x_1, \ldots, x_k) - f_1(x_1^{(i)}, \ldots, x_k^{(i)}) \\ \vdots \\ f_k(x_1, \ldots, x_k) - f_k(x_1^{(i)}, \ldots, x_k^{(i)}) \end{pmatrix}$$
$$- \frac{1}{2} L^{(i)} F_i'' \left(L^{(i)}(F(x) - F(x^{(i)})), L^{(i)}(F(x) - F(x^{(i)})) \right) + \ldots$$

This series development can for each of its k components be written as follows. Denote for $r = 1, \ldots, k$ the function value $f_r(x_1^{(i)}, \ldots, x_k^{(i)})$ by

$f_r^{(i)}$. Then

$$x_j = x_j^{(i)} + \sum_{r=1}^{k} \ell_{jr}^{(i)}(y_r - f_r^{(i)})$$

$$-\frac{1}{2}\sum_{r=1}^{k} \ell_{jr}^{(i)} \sum_{s,t=1}^{k} \left[\frac{\partial^2 f_r(x^{(i)})}{\partial x_s \partial x_t}\left(\sum_{u=1}^{k} \ell_{su}^{(i)}(y_u - f_u^{(i)})\right)\left(\sum_{u=1}^{k} \ell_{tu}^{(i)}(y_u - f_u^{(i)})\right)\right] + \ldots$$

$$= x_j^{(i)} + \sum_{r=1}^{k} c_{\underset{r^{th}\text{ place}}{00,\ldots,\underset{\downarrow}{01},\ldots,00}} (y_r - f_r^{(i)})$$

$$+ \sum_{\substack{s,t=1 \\ s\neq t}}^{k} c_{\underset{s^{th}\text{ and } t^{th}\text{ places}}{00,\ldots,\underset{\downarrow}{01},\ldots,\underset{\downarrow}{01},\ldots,00}} (y_s - f_s^{(i)})(y_t - f_t^{(i)})$$

$$+ \sum_{r=1}^{k} c_{\underset{r^{th}\text{ place}}{00,\ldots,\underset{\downarrow}{02},\ldots,00}} (y_r - f_r^{(i)})^2 + \ldots$$

Using the formulas (I.3.5) for the index sets

$$N = \{(i_1, \ldots, i_k) \mid 1 \leq i_1 + \ldots + i_k \leq 2\} = D$$
$$I = \{(i_1, \ldots, i_k) \mid 1 \leq i_1 + \ldots + i_k \leq 3\}$$
$$H = \{(i_1, \ldots, i_k) \mid i_1 + \ldots + i_k = 3\}$$

we can write down explicit expressions for the numerator and denominator of $[N/D]_I(y_1, \ldots, y_k)$. Making use of section 6 of part I, it is evident that we rediscover Halley's method (II.4.6) by evaluating this expression in the origin

$$[N/D]_I(0, \ldots, 0) = x^{(i)} + \frac{(-L^{(i)}F_i)^2}{-L^{(i)}F_i + \frac{1}{2}L^{(i)}F_i(-L^{(i)}F_i, -L^{(i)}F_i)}$$

The fact that the multivariate Padé approximants introduced in [CUYTd], can be considered as multivariate general order Padé approximants, suggests us to continue our construction of new nonlinear methods because more types of multivariate general order Padé approximants exist. Let us first answer the question "Why?". It is necessary that a number of different techniques exist because the available information of the sytem of nonlinear equations one is dealing with, is not always the same. For formula (II.4.6) all first and second partial derivatives of the functions $f_j(x_1, \ldots, x_k)$, $(j = 1, \ldots, k)$ must be known. This may be a drawback. A completely different situation is encountered in formula (II.5.1). This iterative procedure only uses function evaluations and no derivatives at all. Inbetween lies the iteration we want to introduce here. Suppose some partial derivatives of the $f_j(x_1, \ldots, x_k)$ are given or easily computed. Then from this information the sets N, D and H can be chosen so that precisely these pieces of information are used. Consider for instance for each of the functions $f_j(x_1, \ldots, x_k)$ with $j = 1, \ldots, k$ the same sets N, D and H as in the previous section

$$\begin{aligned} D = N &= \{(0, \ldots, 0), (1, 0, \ldots, 0), \ldots, (0, \ldots, 0, 1)\} \\ H &= \{(2, 0, \ldots, 0), \ldots, (0, \ldots, 0, 2)\} \end{aligned}$$

but now with all interpolation points coinciding. This means that the necessary information to build an iterative procedure with, is

$$\begin{array}{ll} f_j(x_1^{(i)}, \ldots, x_k^{(i)}) & j = 1, \ldots, k \\ \dfrac{\partial f_j}{\partial x_1}(x_1^{(i)}, \ldots, x_k^{(i)}), \ldots, \dfrac{\partial f_j}{\partial x_k}(x_1^{(i)}, \ldots, x_k^{(i)}) & j = 1, \ldots, k \\ \dfrac{\partial^2 f_j}{\partial x_1^2}(x_1^{(i)}, \ldots, x_k^{(i)}), \ldots, \dfrac{\partial^2 f_j}{\partial x_k^2}(x_1^{(i)}, \ldots, x_k^{(i)}) & j = 1, \ldots, k \end{array}$$

The numerator of

$$r_{i_j}(x_1, \ldots, x_k) = \frac{p_{i_j}}{q_{i_j}}(x_1, \ldots, x_k) = \frac{\sum_{(j_1, \ldots, j_k) \in N} a_{j_1 \ldots j_k} x_1^{j_1} \ldots x_k^{j_k}}{\sum_{(j_1, \ldots, j_k) \in D} b_{j_1 \ldots j_k} x_1^{j_1} \ldots x_k^{j_k}}$$

satisfying

$$(f_j q_{i_j} - p_{i_j})(x_1, \ldots, x_k) = \sum_{(\ell_1, \ldots, \ell_k) \in \mathbb{N}^k \setminus (N \cup H)} d_{\ell_1 \ldots \ell_k} x_1^{\ell_1} \ldots x_k^{\ell_k} \tag{II.6.1a}$$

is given by

$$\begin{vmatrix} N_{0\ldots0}(x_1,\ldots,x_k) & N_{10\ldots0}(x_1,\ldots,x_k) & \ldots & N_{0\ldots01}(x_1,\ldots,x_k) \\ \frac{1}{2}\frac{\partial^2 f_j}{\partial x_1^2}(x_1^{(i)},\ldots,x_k^{(i)}) & \frac{\partial f_j}{\partial x_1}(x_1^{(i)},\ldots,x_k^{(i)}) & & 0 \\ \vdots & & \ddots & \\ \frac{1}{2}\frac{\partial^2 f_j}{\partial x_k^2}(x_1^{(i)},\ldots,x_k^{(i)}) & 0 & & \frac{\partial f_j}{\partial x_k}(x_1^{(i)},\ldots,x_k^{(i)}) \end{vmatrix}$$

where

$$N_{i_1\ldots i_k}(x_1,\ldots,x_k) = \sum_{(\ell_1,\ldots,\ell_k)\in N} \frac{\partial^{\ell_1+\ldots+\ell_k-i_1-\ldots-i_k} f_j(x^{(i)})}{\partial x_1^{\ell_1-i_1}\ldots\partial x_k^{\ell_k-i_k}} x_1^{\ell_1}\ldots x_k^{\ell_k}$$

We have of course assumed that the set H provided a system of linearly independent equations. As in the previous section the next iteration step is constructed such that

$$\begin{cases} p_{i_1}(x_1^{(i+1)},\ldots,x_k^{(i+1)}) = 0 \\ \vdots \\ p_{i_k}(x_1^{(i+1)},\ldots,x_k^{(i+1)}) = 0 \end{cases} \qquad (II.6.1b)$$

The numerical behaviour of this method is similar to that of (II.5.1).

Finally we emphasize once more that this section covers in fact a whole bunch of iterative procedures, each adapted to the cost of evaluating and differentiating the nonlinear equations in the system. In the same way as we obtained (II.6.1) we can also set up nonlinear methods based on the use of Canterbury approximants, Karlsson and Wallin approximants, Lutterodt approximants and all types of multivariate general order Padé aproximants that can be described in this framework.

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