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Accelerating the Convergence of a Table with Multiple Entry

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Summary. The idea of using univariate Padé-approximants to accelerate the convergence of a row [6], which can be regarded as a table with single entry, is here generalized: the multivariate Padé-approximants introduced in [2] and briefly repeated in Sect. 1, can be used to accelerate the convergence of a table with multiple entry. In the univariate as well as in the multivariate case the Padé-approximants can be calculated by means of the ε-algorithm [6, 3]. Section 2 treats a table with double entry, while Sect. 3 treats the general case. Numerical examples are given in Sect. 4.

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1. Multivariate Padé-Approximants

In $\mathbb{R}^n$ we write $0=(0, \dots, 0)^t$ and $x=(x_1, \dots, x_n)^t$.

Consider a multivariate real-valued function F, analytic in the origin. In other words

$$\exists r>0: F(x)=\sum_{k=0}^{\infty} \frac{1}{k!} F^{(k)}(0)x^k \quad \text{for } \|x\|<r$$

where $\frac{1}{0!} F^{(0)}(0)x^0 = F(0)$ and $F^{(k)}(0)$ is the k^{th} Fréchet-derivative of F in 0, a symmetric k-linear bounded operator [5, pp. 109–112].

We remind that

$$\frac{1}{k!} F^{(k)}(0)x^k = \sum_{k_1+\dots+k_n=k} \frac{1}{k_1!\dots k_n!} \left.\frac{\partial^k F(x)}{\partial x_1^{k_1} \dots \partial x_n^{k_n}}\right|_{x=0} x_1^{k_1} \dots x_n^{k_n}$$

and that $F(x)=O(x^j)$ if

$$\exists r, J \in \mathbb{R}_0^+, \quad 0<r<1: |F(x)| \leqq J \cdot \|x\|^j \quad \text{for } \|x\|<r.$$

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Definition 1.1. $P(x)=A_m x^m + A_{m-1}x^{m-1}+\ldots+A_1 x + A_0$ where

$$A_0 \in \mathbb{R} \quad \text{and} \quad A_j x^j = \sum_{j_1+\ldots+j_n=j} a_{j_1\ldots j_n} x_1^{j_1}\ldots x_n^{j_n} \quad \text{with } a_{j_1\ldots j_n}\in\mathbb{R}$$

for $j=1,\ldots,m$ is called an *abstract polynomial* [5, p. 111].

Definition 1.2. A couple of abstract polynomials

$$(P_{[l,m]}(x), Q_{[l,m]}(x)) = (A_{lm+l}x^{lm+l}+\ldots+A_{lm}x^{lm},\ B_{lm+m}x^{lm+m}+\ldots+P_{lm}x^{lm})$$

such that the power series $(F\cdot Q_{[l,m]}-P_{[l,m]})(x)=O(x^{lm+l+m+1})$ is called a *solution of the Padé-approximation problem of order* (l,m) *for* F.

Definition 1.3. Let $(P_{[l,m]}(x), Q_{[l,m]}(x))$ be a couple of abstract polynomials satisfying Definition 1.2, with $Q_{[l,m]}(x)\neq 0$. The irreducible form of $\frac{P_{[l,m]}}{Q_{[l,m]}}(x)$ is called the (*abstract*) *multivariate Padé-approximant of order* (l,m) *for* F [2] (abbreviated (l,m) APA).

More details about multivariate Padé-approximants can be found in [2]. For $n=1$ we find back the well-known univariate Padé-approximants.

2. Table with Double Entry

The ε-algorithm has frequently been used to accelerate the convergence of a sequence $(T_i)_{i=0}^{\infty}$ in $\mathbb{R}$ [6], which can in fact be considered as a table with single entry.

Construct the univariate function

$$F(x)=\sum_{i=0}^{\infty} c_i x^i$$

where

$$c_i = T_i - T_{i-1} \qquad (T_i=0 \text{ for } i<0)$$

and calculate the Padé-approximants $\frac{P_{[l,m]}}{Q_{[l,m]}}$ for F.

Since

$$F(1)=\lim_{i\to\infty} T_i$$

one evaluates the Padé-approximants at $x=1$. These values can easily be calculated by means of the ε-algorithm of Wynn [1, pp. 66–68].

If we compute

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

$$\varepsilon_0^{(i)}=\sum_{j=0}^{i} c_j = T_i \qquad i=0,1,\ldots$$

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

$$\varepsilon_{j+1}^{(i)}=\varepsilon_{j-1}^{(i+1)}+\frac{1}{\varepsilon_j^{(i+1)}-\varepsilon_j^{(i)}} \qquad j=0,1,\ldots \text{ and } i=-j,-j+1,\ldots$$

then $\varepsilon_{2m}^{(l-m)}=\frac{P_{[l,m]}}{Q_{[l,m]}}(1)$.

Let us now first consider a table $(T_{ij})_{i,j=0}^{\infty}$ with double entry. To accelerate the convergence of $(T_{ij})_{i,j=0}^{\infty}$ to $\lim_{i,j\to\infty} T_{ij}$ we introduce

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

with

$$c_{ij}=T_{ij}-T_{i,j-1}-T_{i-1,j}+T_{i-1,j-1} \qquad (T_{ij}=0 \text{ for } i<0 \text{ or } j<0).$$

Clearly

$$F(1,1)=\lim_{i,j\to\infty} T_{ij}.$$

We will calculate multivariate Padé-approximants for $F(x,y)$ and evaluate them at $(x,y)=(1,1)$.

If we denote by

$$\tau_i=\sum_{j+k=i} T_{jk}=T_{i,0}+T_{i-1,1}+\ldots+T_{1,i-1}+T_{0,i}$$

and start the ε-algorithm with the partial sums of $F(1,1)$

$$\varepsilon_0^{(i)}=\sum_{j+k=0}^{i} c_{jk}=\tau_i-\tau_{i-1} \qquad i=0,1,\ldots$$

then $\varepsilon_{2m}^{(l-m)}=\frac{P_{[l,m]}}{Q_{[l,m]}}(1,1)$ [3].

An application to accelerate the convergence in quadrature problems will be given in Sect. 4, but first will generalize the idea for a table with multiple entry.

3. Table with Multiple Entry

Let us denote by $(T_{i_1\ldots i_n})_{i_1,\ldots,i_n=0}^{\infty}$ a table with multiple entry. We define

$$F(x_1,\ldots,x_n)=\sum_{i_1,\ldots i_n=0}^{\infty} c_{i_1\ldots i_n}x_1^{i_1}\ldots x_n^{i_n}$$

with

$$\begin{aligned}c_{i_1\ldots i_n}=T_{i_1\ldots i_n}&-\sum_{j=1}^{n} T_{i_1\ldots(i_j-1)\ldots i_n}\\&+\sum_{\substack{j,k=1\\j\neq k}}^{n} T_{i_1\ldots i_{j-1}(i_j-1)i_{j+1}\ldots i_{k-1}(i_k-1)i_{k+1}\ldots i_n}\\&-\ldots+(-1)^n T_{(i_1-1)\ldots(i_n-1)}.\end{aligned}$$

It is easy to prove that

$$F(1,\ldots,1)=\lim_{i_1,\ldots,i_n\to\infty} T_{i_1\ldots i_n}.$$

Again multivariate Padé-approximants for $F(x_1,\ldots,x_n)$ can be calculated and evaluated at $(x_1,\ldots,x_n)=(1,\ldots,1)$ via the ε-algorithm.

Since

$$\sum_{i_1+\ldots+i_n=i} c_{i_1\ldots i_n}=\sum_{j=0}^{n}(-1)^j\binom{n}{j}\tau_{i-j}$$

where

$$\tau_i=\sum_{i_1+\ldots+i_n=i} T_{i_1\ldots i_n}$$

the $\varepsilon_0^{(i)}$ are now given by

$$\varepsilon_0^{(i)}=\sum_{i_1+\ldots+i_n=0}^{i} c_{i_1\ldots i_n}=\sum_{j=0}^{n-1}(-1)^j\binom{n-1}{j}\tau_{i-j}.$$

4. Numerical Results

Suppose one wants to calculate the integral of a function $F(x_1,\ldots,x_n)$ on a bounded closed domain Ω of $\mathbb{R}^n$. Let $\Omega=[0,1]\times\ldots\times[0,1]\subset\mathbb{R}^n$ for the sake of simplicity. The table $(T_{i_1\ldots i_n})_{i_1,\ldots,i_n=0}^{\infty}$ can be obtained for instance by subdividing the interval $[0,1]$ in the j^{th} direction $(j=1,\ldots,n)$ into 2^{i_j} intervals of equal length $h_j=1/2^{i_j}$ $(i_j=0,1,\ldots)$.

Using the midpoint-rule one can then substitute approximations

$$\int_0^{h_1}\ldots\int_0^{h_n} F(x_1,\ldots,x_n)dx_1\ldots dx_n=h_1\ldots h_nF\left(\frac{h_1}{2},\ldots,\frac{h_n}{2}\right)$$

to calculate the $T_{i_1\ldots i_n}$.

The column $\varepsilon_0^{(i)}$ $(i=0,1,\ldots)$ in the ε-table given by

$$\varepsilon_0^{(i)}=\sum_{j=0}^{n-1}(-1)^j\binom{n-1}{j}\tau_{i-j}$$

was also used by Genz [4] to start the ε-algorithm for the approximate calculation of multidimensional integrals by means of extrapolation methods. He preferred this method to six other methods because of its simplicity and general use of fewer integrand evaluations [4]. But when he was using it he did regret that there was no link for the multidimensional problems with Padé-approximants as there is on one dimension. Genz remarked that the construction and theory of the multivariate generalization of Padé-approximants had then only recently been developed by Chisholm and his staff, and that the Canterbury approximants were not particularly suitable for the problem of the extrapolation of sequences of approximations to multiple integrals.

This section has now put things together: the $\varepsilon_0^{(i)}$ are the partial sums of the multivariate function $F(x_1,\ldots,x_n)$ defined in the previous section and the $\varepsilon_{2m}^{(l-m)}$ are the (l,m) APA for that multivariate function, all evaluated in $(x_1,\ldots,x_n)=(1,\ldots,1)$.

We will illustrate everything with some numerical results.

Let us take $n=2$, $h_1=1/2^i$, $h_2=1/2^j$. Then

$$T_{ij}=\frac{1}{2^{i+j}}\left(\sum_{k=1}^{2^i}\sum_{l=1}^{2^j}F\left(\frac{2k-1}{2^{i+1}},\frac{2l-1}{2^{j+1}}\right)\right).$$

For the first example we are going to consider, we have

$$F(x,y)=(x+y)^2$$

$$\int_0^1\int_0^1 F(x,y)\,dx\,dy=7/6=1.1666666\ldots$$

$$T_{00}=1.$$

In Table 4.1 one can find some T_{ij} and some (l,m) APA evaluated in (1, 1). For the calculation of the (l,m) APA we need the τ_i, $i=0,\ldots,l+m$. It is easy to see that the convergence is indeed improved.

Table 4.1

$T_{10}=17/16=1.0625$	(0, 1) APA $=8/7=1.142857142857\ldots$
$T_{11}=\ 9/8\ =1.125$	(1, 1) APA $=7/6=1.1666666\ldots$
$T_{21}=73/64=1.140625$	(2, 1) APA $=7/6=1.1666666\ldots$
$T_{22}=37/32=1.15625$	(3, 1) APA $=7/6=1.1666666\ldots$

What's more: substituting the explicit formula for the T_{ij} in the calculation of the $\varepsilon_0^{(i)}$, one can easily check, using the expressions

$$\sum_{k=1}^{2^i} k^2=\tfrac{1}{3}2^{i-1}(2^i+1)(2^{i+1}+1)$$

and

$$\sum_{k=1}^{2^i} k=2^{i-1}(2^i+1)$$

that for this example $\varepsilon_0^{(i)}=\frac{7}{6}-\frac{1}{6}\cdot(\frac{1}{4})^i$ for $i\geq 0$ which implies [1, p. 45] that the value of the $(i+1,1)$ APA $=\varepsilon_2^{(i)}=7/6$ for $i\geqq 0$.

As a second example we will approximate

$$\int_0^1\int_0^1 \frac{1}{x+y}\,dx\,dy=2\ln 2=1.386294361119891.$$

In Table 4.2 one can again find the T_{ij}, slowly converging to the exact value of the integral because of the singularity of the integrand in (0, 0). The values of the (l,m) APA converge much faster.

Table 4.2

$T_{11}=1.166666666667$	(1, 1) APA $=1.330294906166$
$T_{21}=1.209102009102$	(2, 1) APA $=1.361763927710$
$T_{22}=1.269047619048$	(2, 2) APA $=1.396395820203$
$T_{23}=1.292977663088$	(2, 3) APA $=1.386056820469$
$T_{33}=1.325743700744$	(3, 3) APA $=1.386872037696$
$T_{34}=1.338426108120$	(3, 4) APA $=1.386481238969$
$T_{44}=1.355532404415$	(4, 4) APA $=1.386308917778$
$T_{54}=1.362055745711$	(5, 4) APA $=1.386298323641$

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