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LETTER TO THE EDITOR

Two-variable rational approximants: a new method

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Abstract. A new generalization of Padé approximants to power series in two (or more) variables is given, along with an example of its application.

Considerable interest has been shown in finding two-dimensional generalizations of the Padé approximant scheme. The problem lies in the fact that if we define the numerator and denominator coefficients by requiring

$$\sum_{i=0}^{m}\sum_{j=0}^{m} a_{ij}x^iy^j\left(\sum_{i=0}^{m}\sum_{j=0}^{m} b_{ij}x^iy^j\right)^{-1} = \sum_{k=0}^{N}\sum_{l=0}^{N} c_{kl}x^ky^l \tag{1}$$

be satisfied for some value of N, then the coefficients a_{ij} and b_{ij} are overdetermined. Chisholm (1973) has suggested a scheme which essentially symmetrizes some of the coefficients. Lutterodt (1974) has suggested that a satisfactory method is to ignore some of the defining equations. This letter describes another possibility which might be thought a rather trivial idea were it not for the enormous gain in computational simplicity which it offers.

We start from the ϵ algorithm (Wynn 1956) defined in the following way:

$$\begin{aligned} &\epsilon_m^{(-1)} = 0, \qquad \epsilon_m^{(0)} = \sum_{k=0}^{m} c_kx^k \qquad m \leqslant N \\ &\epsilon_m^{(j+1)} = \epsilon_{m+1}^{(j-1)} + 1/(\epsilon_{m+1}^{(j)} - \epsilon_m^{(j)}). \end{aligned} \tag{2}$$

As is well known, the ϵ algorithm is related to the Padé table via

$$\epsilon_m^{(2k)} = [k+m, k] = P_{k+m}(x)/Q_k(x). \tag{3}$$

In other words, it offers an exceptionally simple way of evaluating Padé approximants, and it appears to be numerically more stable than either the methods proposed by Baker (1970) or Watson (1973). The generalization we propose is to write

$$\epsilon_m^{(0)} = \sum_{k=0}^{m}\sum_{j=0}^{m} c_{kj}x^ky^j \tag{4}$$

(the generalization to several variables is obvious).

The algorithm (2), modified by (4) then provides a stable, simple rational approximation to the function of two variables defined by the power series. It satisfies the canonical requirements that it reduces to the conventional single-variable expression if the second variable is put equal to zero and that it is symmetrical in x and y if the original function is. As a simple example of its use, we consider the kind of problem which might arise in critical phenomena (see, eg, Wood and Griffiths 1974). We have used the algorithm in a computer search for the poles of the function

$$f(x, y) = \frac{1}{e^{xy} - y} = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} c_{ij} x^i y^j \tag{5}$$

considered as a function of x. Table 1 shows the values of x obtained via the algorithm (with $N = 8$) compared to the exact result

$$x = \frac{1}{y} \ln y \tag{6}$$

for a range of values of y. The results are obviously satisfactory. Straightforward computational precautions must be taken to avoid the possibility of

$$\epsilon_{m+1}^{(j)} = \epsilon_m^{(j)}$$

for some m and j: this is analogous to the Padé table being non-normal.

Table 1.

y	x_0†	δx‡
0·5	−1·3863	$8{\cdot}2 \times 10^{-6}$
1·0	0	$2 \times 10^{-1{\cdot}6}$
1·5	0·2703	$6{\cdot}1 \times 10^{-8}$
2·0	0·3466	$1{\cdot}5 \times 10^{-6}$
2·5	0·3685	$7{\cdot}6 \times 10^{-6}$
3·0	0·3662	$2{\cdot}2 \times 10^{-5}$
3·5	0·3579	$4{\cdot}6 \times 10^{-5}$
4·0	0·3466	$8{\cdot}2 \times 10^{-5}$
4·5	0·3342	$1{\cdot}3 \times 10^{-4}$
5·0	0·3219	$1{\cdot}9 \times 10^{-4}$

† x_0 is the exact position of the pole, given by (6).
‡ δx is the proportional error in the position as calculated by the algorithm.

The algorithm is an interesting insight as to the 'natural' generalization of Padé approximants. If we consider the truncated series

$$f(x, y) = \sum_{i=0}^{2} \sum_{j=0}^{2} c_{ij} x^i y^j \tag{7}$$

then we find from (4) and (2)

$$\epsilon_0^{(2)} = \frac{\hat{P}(x, y)}{\hat{Q}(x, y)} \tag{8}$$

where $\hat{P}$, $\hat{Q}$ are polynomials of the form

$$\hat{P}(x, y) = p_{10}x + p_{01}y + p_{11}xy + p_{20}x^2 + p_{21}x^2y + p_{22}x^2y^2 + p_{12}xy^2 + p_{02}y^2 \tag{9}$$

and the p_{ij} are simply expressible as functions of the c_{ij}. This implies that we require 15 coefficients (the overall normalization may be fixed by putting $q_{01} = 1$) to describe a power series with only 9 terms: in other words in addition to the 9 equations to define the p_{ij} and q_{ij} in terms of the c_{ij}, we require an additional 6 equations to eliminate this redundancy. The ϵ algorithm, of course, avoids this problem entirely.

An alternative method of using the ϵ algorithm in a two-variable problem is the following: we define the subfunctions (for all $k \leqslant N$)

$$f_k(y) = \sum_{j=0}^{\infty} c_{kj} y^j, \qquad \epsilon_m^{(0)(k)} = \sum_{j=0}^{m} c_{kj} y^j$$
$$b_k = \epsilon_0^{(2m)(k)}, \qquad \epsilon_l^0 = \sum_{k=0}^{l} b_k x^k. \tag{10}$$

That is, we form a series of approximants in one variable, and use this to create a Taylor series in the second. The method is numerically satisfactory for some problems; however, it fails on two counts. Firstly, the result is *not* a rational approximation in two variables, but rather a rational approximation in one variable whose coefficients are rational approximations in the second. Secondly, it is possible for the subfunctions defined in (10) to have singularities which bear no relation to the singularities of the full function. This actually occurs in our example (5), where

$$c_{0j} = 1 \qquad \text{(all } j\text{)}$$

implying an apparent singularity at $y = 1$, which is subsequently cancelled by singularities in other subfunctions.

It is perhaps of interest to mention a method of defining the two-dimensional analogue of Padé approximants of the second kind (see eg Genz 1973), defined via

$$\sum_{i=0}^{m} p_i x_l^i \left(\sum_{i=0}^{m} q_i x_l^i \right)^{-1} = f(x_l) \tag{11}$$

for a series of values x_l. Fixing $y = y_m$, we can find a series of one-dimensional Padé approximants (most conveniently from Thiele's method), giving

$$\sum_{i=0}^{N} p_i^{(m)} x^i \left(\sum_{i=0}^{N} q_j^{(m)} x^j \right)^{-1} = f(x, y_m). \tag{12}$$

We can now regard the $p_i^{(m)}$ and $q_i^{(m)}$ as functions of y: to maintain the approximation as a rational one it is necessary that they be treated as polynomials

$$p_i^{(m)} = p_i(y_m) = \sum p_{ij} y_m^{\gamma} \tag{13}$$

and the coefficients may be evaluated using Erskine's (1956) method. Applications of this method will be discussed at greater length in a future paper.

In addition to the applications of these methods in critical phenomena, they may be of use in the evaluation of Feynman graphs, where Kershaw (1973) has shown that certain important classes of graphs give rise to multi-variable power series.

Note added in proof. Dr P Graves-Morris has suggested (private communication) that an alternative to (4) would be to write

$$\epsilon_m^{(0)} = \sum_{k=0}^{m} \sum_{j=0}^{k} c_{m-k,j} x^{m-k} y^j. \tag{4'}$$

This appears to be as satisfactory, and is perhaps a rather more elegant generalization.

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