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The Epsilon algorithm and operational formulas of numerical
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The Epsilon Algorithm and Operational Formulas of Numerical Analysis

By P. Wynn

1. Introduction. It is the purpose of this paper to describe a non-linear technique which appears to have powerful and general application in numerical analysis. However, before doing so it is necessary to refer to a few related theoretical concepts.

2. Rational Operational Formulas. The double sequence of rational functions

$$\frac{U_{\mu,\nu}(x)}{V_{\mu,\nu}(x)} \quad \mu, \nu = 0, 1, \dots$$

where

$$(1) \quad \frac{U_{\mu,\nu}(x)}{V_{\mu,\nu}(x)} = \frac{\alpha_{\mu,\nu,0} + \alpha_{\mu,\nu,1}x + \dots + \alpha_{\mu,\nu,\nu}x^\nu}{\beta_{\mu,\nu,0} + \beta_{\mu,\nu,1}x + \dots + \beta_{\mu,\nu,\mu}x^\mu}$$

may be derived from the series

$$(2) \quad \beta(x) = \sum_{s=0}^{\infty} c_s x^s$$

by imposing the condition that the power series expansion of (1) should agree with (2) as far as the term in $x^{\mu+\nu}$. If none of the Hankel determinants

$$\begin{vmatrix} c_m & c_{m+1} & \dots & c_{m+k-1} \\ c_{m+1} & c_{m+2} & \dots & c_{m+k} \\ \vdots & \vdots & & \vdots \\ c_{m+k-1} & c_{m+k} & \dots & c_{m+2k-2} \end{vmatrix} \quad m, k-1 = 0, 1, \dots$$

vanish, and the additional condition $\beta_{\mu,\nu,0} = 1$ is imposed, the coefficients in the rational expression (1) are uniquely determined. The rational expressions (1) may be placed in a two-dimensional array in which the quotient (1) occurs at the intersection of the $(\mu+1)$ th row and the $(\nu+1)$ th column. [1] [2] [3].

As is well known, the numerical convergence of the sequence

$$(3) \quad \frac{U_{r,r}(x)}{V_{r,r}(x)} \quad r = 0, 1, \dots$$

for a particular value of x is in many cases much better than that of the series (2). This consideration led Kopal [4] to the consideration of rational operational formulas, that is, to the replacement of the operational equation

$$(4) \quad \left(\sum_{s=0}^{\infty} c_s d^s \right) F = f$$

where F is a known function from which f is to be determined, and d is a finite dis-

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placement operator, by the equation

$$(5) \quad \left(\frac{U_{r,r}(d)}{V_{r,r}(d)} \right) F = f.$$

Equation (5) cannot at the moment, in its non-linear form, be solved. The equation may however be linearized by multiplication throughout by $V_{r,r}(d)$ to give

$$(6) \quad U_{r,r}(d)F = V_{r,r}(d)f.$$

Assuming that F and f are completely known, that r in equation (6) is sufficiently large, and the example is a suitable one, then there will exist considerable numerical agreement between the right and left hand sides of equation (6). Assuming that d is any one of the conventional operators Δ , E , ∇ , μ , δ of numerical analysis, and that F and the sequences of values $f_1, f_2, \dots; f_{-1}, f_{-2}, \dots$ are known, then equation (6) may be rearranged so as to determine f_0 . It is this very last assumption which constitutes a serious limitation of the linearizing technique resulting in equation (6). Indeed, Kopal was only able to find useful application of the technique when d was the backward difference operator, though his numerical results, which related to the forward integration of a differential equation, appeared to be very promising. However, the same effect over a very much larger range of problems may be achieved by recourse to another method.

3. The $e_m(S_n)$ Transformation. In his researches into the non-linear transformation*

$$(7) \quad e_m(S_n) = \frac{\begin{vmatrix} S_n & S_{n+1} & \cdots & S_{n+m} \\ \Delta S_n & \Delta S_{n+1} & \cdots & \Delta S_{n+m} \\ \vdots & \vdots & \cdots & \vdots \\ \Delta S_{n+m-1} & \Delta S_{n+m} & \cdots & \Delta S_{n+2m-1} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \cdots & 1 \\ \Delta S_n & \Delta S_{n+1} & \cdots & \Delta S_{n+m} \\ \vdots & \vdots & \cdots & \vdots \\ \Delta S_{n+m-1} & \Delta S_{n+m} & \cdots & \Delta S_{n+2m-1} \end{vmatrix}} \quad m, n = 0, 1, \dots$$

of the sequence $S_r, r = 0, 1, \dots$ Shanks [5], by an appeal to the theory of linear equations, showed that if

$$(8) \quad S_r = \sum_{s=0}^r c_s x^s \quad r = 0, 1, \dots$$

then

$$(9) \quad e_m(S_n) = \frac{U_{m,m+n}(x)}{V_{m,m+n}(x)} \quad m, n = 0, 1, \dots$$

The same result may be derived from the theory of orthogonal polynomials [6].

4. The ϵ -Algorithm. The evaluation of the determinants in the various expressions (7) is sufficiently laborious to be prohibitive. However, the expressions (7)

* The notation used here is consistent with that of [7] but differs slightly from that of [5] where the right hand side of (7) would be designated as $e_m(S_{n+m})$.

may be computed recursively by means of the ϵ -Algorithm as follows [7]. If, from the initial conditions

$$(10) \quad \epsilon_{-1}^{(m)} = 0 \quad m = 1, 2, \dots; \quad \epsilon_0^{(m)} = S_m \quad m = 0, 1, \dots$$

quantities $\epsilon_s^{(m)}$ are computed recursively using the relation

$$(11) \quad \epsilon_{s+1}^{(m)} = \epsilon_{s-1}^{(m+1)} + \frac{1}{\epsilon_s^{(m+1)} - \epsilon_s^{(m)}} \quad m, s = 0, 1, \dots,$$

then

$$(12) \quad \epsilon_{2s+1}^{(m)} = \{e_s(\Delta S_m)\}^{-1} \quad \epsilon_{2s}^{(m)} = e_s(S_m) \quad m, s = 0, 1, \dots$$

If the quantities $\epsilon_s^{(m)}$ are arranged in the scheme

$$\begin{array}{ccccccc} & & \epsilon_0^{(0)} & & & & \\ \epsilon_{-1}^{(1)} & & & \epsilon_1^{(0)} & & & \\ & \epsilon_0^{(1)} & & & \cdot & & \\ \epsilon_{-1}^{(2)} & & \epsilon_1^{(1)} & & & \cdot & \epsilon_s^{(0)} \\ & \epsilon_0^{(2)} & & & \cdot & & \epsilon_{s+1}^{(0)} \\ \epsilon_{-1}^{(3)} & & \epsilon_1^{(2)} & & & \cdot & \epsilon_s^{(1)} \\ & \epsilon_0^{(3)} & & & \cdot & & \epsilon_{s+1}^{(1)} \\ \vdots & \vdots & \vdots & & & \cdot & \epsilon_s^{(2)} \\ & & & & & & \epsilon_{s+1}^{(2)} \\ & & & & & & \vdots \end{array}$$

it will be seen that relations (11) may be used, column by column, to build up the scheme from left to right. It should be noted that if conformity, by means of equations (9) and (12), is to take place between the Padé Table and the ϵ -array, the latter must be transposed about the diagonal $m = 0$; the columns of the ϵ -array with even order suffixes then take their place as rows in the Padé Table.

The following theorem, based upon the results of the last two sections, may now be given:

THEOREM. *If p is an associative and commutative operator, and*

$$(13) \quad a_s p^s F = c_s x^s \quad s = 0, 1, \dots$$

and quantities $\epsilon_s^{(m)}$ are computed using the relation (11) from the initial values

$$(14) \quad \epsilon_{-1}^{(m)} = 0 \quad m = 1, 2, \dots; \quad \epsilon_0^{(m)} = \sum_{s=0}^m a_s p^s F$$

then

$$(15) \quad \epsilon_{2s}^{(m)} = \frac{U_{s, m+s}(x)}{V_{s, m+s}(x)} \quad m, s = 0, 1, \dots$$

FIRST EXAMPLE: A numerical example of the application of the theorem now follows. It concerns the process of obtaining the derivative at $z = 0$ of the function $\exp(hz)$, when $h = 0.6$, by means of the formula

$$(16) \quad \left(\frac{d}{dz} F \right)_{z=0} = \sum_{s=0}^{\infty} \frac{(-1)^s}{s+1} \Delta^{s+1} F.$$

Here, in the notation of equation (13)

$$(17) \quad \frac{(-1)^s}{(s+1)} \Delta^{s+1} F = \frac{(-1)^s}{(s+1)} (e^h - 1)^{s+1}.$$

The quantities with even order suffix in the ϵ -array for this example are displayed in Table I.

Note: The results of Table I begin with the diagonal $m = 1$. If the notation of equation (15) is strictly to be adhered to, an entry $\epsilon_0^{(0)} = 0$ together with a corresponding diagonal should be appended to Table I. However, this is not a matter of great importance, and in the event that an operational series were to begin with a term in $p^s, s > 1$, even this artifice would not be available.

It is perhaps in order to comment upon the power of the algorithm as revealed by this example. Attainment of the same accuracy as is achieved in Table I by the straightforward use of the series (16), even neglecting the accumulation of round-off errors, would involve the summation of about eighty terms and an excursion into arithmetic involving twenty-eight decimal figures.

The Padé quotients (3) in this example are successive convergents of the continued fraction

$$(18) \quad x^{-1} \log(1+x) = \frac{1}{1+} \frac{1^2x}{2+} \frac{1^2x}{3+} \frac{2^2x}{4+} \frac{2^2x}{5+} \dots$$

Numerical investigation into the behavior of this continued fraction [8] shows that application of the ϵ -algorithm to the series (16) converges quite reasonably for $(e^{hz} - 1) > 1$, when the series rapidly diverges.

In the derivation of the classical operational formulas of numerical analysis the operand is assumed to be a polynomial, and the formulas derived are then completely valid. The formulas are then universally applied, without examination of the operand, and without any more justification than that of the results achieved.

In the same way it occurs that although formula (13) is no longer valid, use of the ϵ -algorithm in conjunction with operational series meets with success. Two examples which support this thesis now follow.

SECOND EXAMPLE: This concerns the interpolation of the function $\log(0.6 + hz)$ when $h = 0.1$ and $z = 0.25$ with points of tabulation at unit intervals of z , by use

TABLE I

0.8221 1880						
0.4841 7914	0.6038 2270					
0.6693 9684	0.5987 5229	0.6000 7869				
0.5551 9362	0.6005 0406	0.5999 7937	0.6000 0168			
0.6303 0451	0.5997 6720	0.6000 0665	0.5999 9961	0.6000 0004		
0.5788 4612	0.6001 1785	0.5999 9752	0.6000 0011	0.5999 9999	0.6000 0000	
0.6151 0747	0.5999 3622	0.6000 0102	0.5999 9996	0.6000 0000		
0.5890 2272	0.6000 3631	0.5999 9954	0.6000 0001			
0.6080 8473	0.5999 7849	0.6000 0022				
0.5939 8062	0.6000 1316					
0.6045 2176						

of Bessel's Interpolation Formula

$$(19) \quad F(z) = \sum_{s=0}^{\infty} a_s F(0)$$

where

$$(20) \quad \begin{aligned} a_0 &= 1 & a_1 &= z\delta E^{1/2} \\ a_{2s} &= \binom{2+s-1}{2s} \mu \delta^{2s} E^{1/2}, \\ a_{2s+1} &= \frac{z - \frac{1}{2}}{2s+1} \binom{2+s-1}{2s} \delta^{2s+1} E^{1/2} s = 1, 2, \dots \end{aligned}$$

The quantities $\epsilon_s^{(m)}$ with even order suffix are displayed in Table II.

Since $\log(0.625) = -0.4700\ 036$, it will be seen that application of the ϵ -algorithm results in an effective gain of three decimal figures. This is not spectacular, but there is no point in selecting for presentation only those examples which display the method in a particularly favorable light. It might be mentioned at this point that the author has experimented with the ϵ -algorithm in conjunction with operational formulas in a large number of cases, and in none of these was the accuracy of the transformed results worse than the original partial sums.

Since the odd and even order terms in the series (19) are so dissimilar, the odd and even terms were separated out and the two series submitted separately to treatment by the ϵ -algorithm, the transformed results subsequently being added together. The numerical results produced in this way were not, however, significantly better than those shown in Table II.

THIRD EXAMPLE: This concerns the application of the Euler-Maclaurin integration formula

$$(21) \quad \int_x^{x+h} F(t) dt = \frac{h}{2} \{F(x) + F(x+h)\} - \sum_{s=1}^m \frac{h^{2s+1} B_{2s}}{(2s)!} \Delta_h F^{(2s-1)}(x)$$

when the integrand is the function $\exp(-z^2)$ and the upper and lower limits of integration are 0 and $w(1+i)$ respectively, with $w = 0.75$.

The functions $u_s = \frac{h^{s+2} F^{(s)}(h)}{(s+1)!}$ in this example satisfy the recursion

$$(22) \quad s(s+1)u_s + 2h^2 s u_{s-1} + 2h^2 (s-1)u_{s-2} = 0$$

TABLE II

-0.4337 503				
0.4722 880	-0.4701 290			
0.4700 009	0.4699 404	-0.4699 923		
0.4699 419	0.4699 732	0.4700 085	-0.4700 040	
0.4700 084	0.4700 105	0.4700 032	0.4700 027	-0.4700 034
0.4700 105	0.4700 088	0.4700 027	-0.4700 031	
0.4700 020	0.4700 017	0.4700 040		
0.4700 017	-0.4700 019			
-0.4700 048				

TABLE III

0.875 042 + $i0.198\ 341$	0.921 529 + $i0.408\ 848$	0.917 213 + $i0.403\ 098$	0.917 256 + $i0.403\ 708$		
0.941 289 0.385 856	0.915 669 0.404 484	0.917 498 0.403 703	0.917 299 0.403 626	0.917 318 + $i0.403\ 659$	
0.925 783 0.409 131	0.917 028 0.402 979	0.917 258 0.403 730	0.917 321 0.403 657	0.917 302 0.403 657	
0.915 984 0.408 382	0.917 657 0.403 511	0.917 271 0.403 620	0.917 302 0.403 661	0.917 306 + $i0.403\ 651$	0.917 307 + $i0.403\ 652$
0.914 273 0.403 627	0.917 403 0.403 874	0.917 332 0.403 635	0.917 303 + $i0.403\ 650$		
0.916 792 0.401 460	0.917 147 0.403 734	0.917 319 0.403 675			
0.919 060 0.402 800	0.917 231 0.408 522	0.917 289 + $i0.403\ 663$			
0.918 494 0.405 171	0.917 427 0.403 573				
0.915 922 0.405 283	0.917 403 + $i0.403\ 776$				
0.915 008 0.402 370					
0.918 429 + $i0.400\ 273$					

with

$$(23) \quad \begin{aligned} u_0 &= -w\{\cos(2w^2) + \sin(2w^2)\} - iw\{\cos(2w^2) - \sin(2w^2)\} \\ u_1 &= -2w^3\{\cos(2w^2) - \sin(2w^2)\} + i2w^3\{\cos(2w^2) + \sin(2w^2)\}. \end{aligned}$$

The quantities $\epsilon_s^{(m)}$ (which are now complex numbers) with even order suffix are displayed in Table III. Since $\operatorname{erf}(0.75(1+i)) = 0.917\,306 + i0.403\,654$, application of the ϵ -algorithm has in this case resulted in the gain of about three decimal places.

It is perhaps of interest to point out that the accuracy of the transformed results produced in the first and third examples could have been increased by extending the computation. This is also true to a limited extent of the second example, but the non-existence of central differences above a certain order limits the extent to which the computation may be prolonged.

It would be useful, when examining the mathematical validity of the procedures adopted in the second and third examples, to be able to relate the determinantal quotient

$$\begin{vmatrix} \sum_{s=0}^{s=0} c_s p^s F & \sum_{s=0}^{s=1} c_s p^s F & \cdots & \sum_{s=0}^{s=m} c_s p^s F \\ c_1 p^1 F & c_2 p^2 F & \cdots & c_{m+1} p^{m+1} F \\ \vdots & \vdots & \cdots & \vdots \\ c_m p^m F & c_{m+1} p^{m+1} F & \cdots & c_{2m} p^{2m} F \end{vmatrix}$$

$$\begin{vmatrix} 1 & 1 & \cdots & 1 \\ c_1 p^1 F & c_2 p^2 F & \cdots & c_{m+1} p^{m+1} F \\ \vdots & \vdots & \cdots & \vdots \\ c_m p^m F & c_{m+1} p^{m+1} F & \cdots & c_{2m} p^{2m} F \end{vmatrix}$$

to the solution f of the operational equation

$$\sum_{s=0}^{\infty} c_s p^s F = f,$$

but this appears to be one of the cases in which a statement of the problem is not a great step forward to its solution.

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