

Algorithms

G. E. FORSYTHE, Editor

ALGORITHM 234

POISSON-CHARLIER POLYNOMIALS [S23]

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real procedure *PCpolynomial* (*x*, *n*, *a*);

integer *n*; **real** *x*, *a*;

comment *PCpolynomial* computes values of the Poisson-Charlier polynomial $p_n(x)$ defined by L. Carlitz, Characterization of certain sequences of orthogonal polynomials, *Portugaliae Mathematica* 20 (1961), 43-46:

$$p_n(x) = a^{n/2}(n!)^{-1/2} \sum_{r=0}^n (-1)^{n-r} \binom{n}{r} r! a^{-r} \binom{x}{r}.$$

In this algorithm *u* stands for the successive terms of the summation, *s* stands for the sum of these terms and all other symbols possess evident meanings. Clearly each term of the summation is obtained from the preceding one by the indicated multiplication;

begin

integer *j*; **real** *u*, *s*, *c*;

u := (-1) ↑ *n*;

s := *u*;

c := 1;

for *j* := 1 **step** 1 **until** *n* **do** *c* := *c* × *j*;

for *j* := 0 **step** 1 **until** *n* - 1 **do**

begin *u* := - *u* × (*n* - *j*) × (*x* - *j*) / (*a* × (*j* + 1)); *s* := *s* + *u* **end**;

PCpolynomial := *sqr*t(*a* ↑ *n* / *c*) × *s*

end *PCpolynomial*

ALGORITHM 235

RANDOM PERMUTATION [G6]

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procedure *SHUFFLE* (*a*, *n*, *random*);

value *n*; **integer** *n*; **real procedure** *random*; **integer**

array *a*;

begin

comment *SHUFFLE* applies a random permutation to the sequence $a[i]$ where $i = 1, 2, \dots, n$. The procedure *random* is supposed to supply a random element from a large population of real numbers uniformly distributed over the open unit interval $0 < r < 1$. The array *a* is declared to be integer but actually it suffices for its type to agree with that of the variable *b* (in the procedure body);

integer *i*, *j*; **real** *b*;

for *i* := *n* **step** - 1 **until** 2 **do**

begin *j* := *entier* (*i* × *random* + 1);

b := *a*[*i*]; *a*[*i*] := *a*[*j*]; *a*[*j*] := *b*

end **loop** *i*

end *SHUFFLE*

Note. Numbers in brackets following Algorithm titles indicate the subject category for the algorithm, based on the Modified SHARE Classification listing given in the March, 1964 issue of the *Communications of the ACM*.

REMARK ON ALGORITHM 60 [D1]

ROMBERG INTEGRATION [F. L. Bauer, *Comm. ACM* 4 (June 1961) 255; 5 (Mar. 1962), 168; 5 (May 1962), 281]

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* Work supported by the U. S. Atomic Energy Commission.

The Romberg integration algorithm has been used with great success by many groups [1, 2], and appears to be among the most generally reliable quadrature methods available. It is, therefore, worth pointing out that it is not entirely foolproof, and that a significant class of integrands exists for which the extrapolated values are poorer estimates of the integral than the corresponding trapezoidal sums.

The validity of the Romberg procedure depends upon the possibility of expanding the error of the trapezoidal rule in powers of h^2 , where h is the stepsize. One expansion of this type is the Euler-Maclaurin sum formula. An alternative expression may be obtained from the Fourier series expansion. The coefficients of h^{2r} in the Euler-Maclaurin formula are proportional to the difference of the values of the $(2r+1)$ -th derivative at the two ends of the range. Thus, any integral for which the odd derivatives of the integrand either vanish or are equal at the limits will not be improved by Romberg extrapolation. Among the common examples of such integrals are integrals of periodic functions over a period and integrals for which the derivatives vanish at both limits. An example of the last type is the integral approximation to the modified Hankel function [3], $e^x K_p(x) = \int_0^L e^{x(1-\cosh t)} \cosh(pt) dt$, where L is taken so large that the contribution of the integral from L to ∞ may be neglected. Several other examples are given under the heading "Exceptional cases" by Bauer, Rutishauser and Stiefel [7]. This paper is among the most extensive discussions of the Romberg method in English.

The algorithm also fails when the expansion of the error term contains other powers of h along with the even ones. Rutishauser [4] discusses estimating integrals of the form $\int_0^a f(x) dx = \int_0^a (\varphi(x)/\sqrt{x}) dx$. If such integrals are estimated by the trapezoidal rule, assigning the value 0 to $f(0)$, the error may be expressed in the form $\sum c_k h^{2k} + \sqrt{h} \sum d_k h^k$. Although the standard Romberg extrapolation fails when applied to this sequence of estimates, Rutishauser presents a modified procedure which is effective.

The extrapolation is also invalid when the integrand is discontinuous, although this exception is trivial from the computational standpoint.

It has also been pointed out [5, 6] that the Romberg procedure may amplify round-off errors. The losses, while significant, do not appear prohibitive for most applications.

REFERENCES:

1. THACHER, H. C., JR. Certification of algorithm 60. *Comm. ACM* 5 (Mar. 1962), 168.
2. BUCHNER, K. H. Certification of algorithm 60. *Comm. ACM* 5 (May, 1962), 281.
3. FETTIS, H. E. Algorithm 163, modified Hankel function. *Comm. ACM* 6 (Apr. 1963), 161-2; 6 (Sep. 1963), 522.

4. RUTISHAUSER, H. Ausdehnung des Rombergschen Prinzips. *Numer. Math.* 5 (1963), 48-54.
5. McKEEMAN, W. M. Personal communication, Sept. 1963.
6. ENGEL, M. Personal communication, Jan. 1964.
7. BAUER, F. L., RUTISHAUSER, H., AND STIEFELE, E. New aspects in numerical quadrature. *Proc. Symp. Appl. Math* 15, 1963, 199-218.

CERTIFICATION OF ALGORITHM 128 [C6]
SUMMATION OF FOURIER SERIES [M. Wells, *Comm. ACM* 5 (Oct. 1962), 513]

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The body of *Fourier* was transcribed for the Dartmouth SCALP translator for the LGP-30 computer. After uniformizing the spelling of *zeros* (lines 5 and 9 in the procedure body), the program compiled and ran without difficulty.

In the procedure statement for *Fourier*, the actual parameter corresponding to *X* should be an expression depending on the actual parameter corresponding to *r*.

The SCALP program was tested for the finite series:

$$A = \sum_{r=0}^{n-1} \cos rw = \frac{\sin((n-1)w/2)}{\sin(w/2)} \cos(nw/2) + 1$$

$$B = \sum_{r=0}^{n-1} \sin rw = \frac{\sin((n-1)w/2)}{\sin(w/2)} \sin(nw/2)$$

for $w = 0.1, 0.2, 0.5$ and 1.0 , and for $n = 1(1)51$. Although the algorithm appears to be numerically correct, the results showed evidence of serious numerical instability, particularly for small values of w . For $w = 0.1$, and $n = 51$, the error in A was .00109, and in B , -.00231. Since the largest A for $n < 51$ is 10.5, and the largest B about 20, the best result obtainable with the 7+ significant digit arithmetic of the SCALP system is about .00001. For comparison, a program summing the same series using a forward recurrence based on the addition formulas for the sine and cosine gave errors of .00012 and -.00018. It was, however, only about half as fast.

REMARK ON ALGORITHM 135 [F4]
CROUT WITH EQUILIBRATION AND ITERATION
[W. M. McKeeman, *Comm. ACM* 5 (Nov. 1962), 555-557, 559]

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The following corrections to the published algorithm are recommended:

1. Two lines above the bottom line of procedure *SOLVE* one must change

$$y[k] := t \quad \text{to} \quad y[k] := t/A[k,k]$$

2. In procedure *EQUILIBRATE*, all occurrences of the subscript k must be changed to j .

3. The statement $cnr := 1.0$ should be added at the start of the body of procedure *LINEARSYSTEM*, so that cnr will have a value the first time it is used.

4. Line 19 from the end of *LINEARSYSTEM* should be changed from

if normdy = 0 then begin cnr := 1.0; go to enditer end;

to read

if normdy = 0 then go to enditer;

This correction makes sure that cnr retains a reasonable value in case $normdy$ should be 0 for some column.

5. The symbol “.” must be removed from the parameter delimiters in the declarations of procedures *LINEARSYSTEM*, *RESIDUALS* and *SOLVE*.

6. Four lines above the bottom line of procedure *LINEARSYSTEM*, delete the first occurrence of $X[i,k] :=$

7. In the third line of the heading of procedure *IP2*, the parameter delimiter

) extra term:(

should be changed to

) extra term:(

CERTIFICATION OF ALGORITHM 170 [F3]
REDUCTION OF A MATRIX CONTAINING POLYNOMIAL ELEMENTS [P. E. Hennion, *Comm. ACM* 6 (April 1963), 165; 6 (Aug. 1963), 450]
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Algorithm 170 was translated into FAST for the NCR 315 and gave satisfactory results with the following corrections:

1. **real procedure ... integer NCOL, N;** should be replaced by

**procedure POLYMATRIX (A, NCOL, N, COE, NP1);
value NCOL, N; real array A, COE;
integer NCOL, N, NP1;**

2. At the end of the first comment add:

The global integer procedure *MAX* is assumed and furnishes the maximum of two integers.

3. **integer i, j, k, ... COE[1:M];**

should be replaced by

**integer i, j, k, j1, j2, j3, j4, j5, j6, j7, j8, j9, j10, j11, M;
array C1, C2[1:N×NCOL+1];**

4. Immediately after *start*: the statement

$NP1 := N + 1;$

should be added, and the third line after *start*: i.e.,

for k := 1 step 1 until M do begin

should be replaced by

for k := 1 step 1 until NP1 do begin

5. The third line after *L10*: i.e.,

for k := 1 step 1 until M do ...

should be replaced by

for k := 1 step 1 until j7 do ...

The last two changes simply shorten both of the indicated *for* statements.

[EDITOR'S NOTE. In addition to the above corrections, we have two comments on the Remark on Algorithm 170 by Hennion, *loc. cit.*, p. 450:

First, the semicolon at the end of the first line after *L0* must be removed.

Second, correction (4) is irrelevant.

The referee confirms that a transcription into Burroughs Extended ALGOL of the program as corrected by Mrs. Pribe runs on the B5000.—G.E.F.]