Coefficients for numerical integration as defined by Pickard

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Abstract

The definition of some integer sequences and triangles in [6], and the relationship between these definitions, and some similar notions in other works on numerical integration, is a little unclear. We try to make the definitions precise and to provide a concordance with other notations.

The two methods of numerical solution of ODEs which these coefficients are used in is explained in [6] as well as in [1] and [5]. Here, we are not concerned with explicating this method, but only with the correct calculation of the coefficients.

1 Pickard's paper

1.1 $\aleph_j$ and $\aleph_j^\star$

The article [6] provided the sequences A002397 to A002406 as well as A260780 and A260781. Most of these sequences are taken from the tables for $\delta_p(J)$ and $\delta_p^\star(J)$. These are defined for all $0 \leq J$ and $0 \leq p \leq J$.

Pickard first defines (in equation (6a)):

$$\beta_j = \frac{1}{j!} \int_0^1 (u + j - 1)^{[j]} du \tag{1}$$

where the integrand is the polynomial defined by:

$$(u - l)^{[j]} = (u - l)(u - l - 1) \cdots (u - l - j + 1)$$

The goal is to use β_j in the estimate:

$$y(x_1) = y(x_0) + h \sum_{j=0}^{J} \beta_j \Delta^j f_{-j} + E_J$$

where E_J is an error term, and Δ is a forward difference operator.

The polynomial has integer coefficients and highest term u^j. Thus the integral between 0 and 1 is a sum of fractions with denominators $1, 2, \ldots (j+1)$. So it can be written as a fraction with denominator $L(j) =$

gcd$(1, 2, \ldots, (j+1))$. Thus the denominator of β_j divides $L(j)j!$, and Pickard defines an integer sequence

$$\aleph_j = L(j)j!\beta_j \tag{2}$$

Thus the $\aleph_j$ can be worked out mechanically, either from the definite integral (1), or using the Stirling numbers, which comes to the same thing, and thence the integer sequences $\aleph_j$ and $L(j)j!$ give the rational sequence β_j as their ratio. There is some uncertainty, which we have not attempted in this work to resolve, about the 'generalized Stirling numbers of the first kind'. The intended definition is clear from Pickard's usage. To avoid ambiguity, we used the integral definition (1) only to work with β_j.

An entirely analogous set of definitions give $\beta_j^\star$ and $\aleph_j^\star$:

$$\beta_j^\star = \frac{1}{j!}\int_{-1}^{0}(u+j-1)^{[j]}du$$

$$\aleph_j^\star = L(j)j!\beta_j^\star$$

$$y(x_0) = y(x_1) + h\sum_{j=0}^{J}\beta_j^\star \Delta^j f_{-j} + E_J^\star$$

Here the only difference between these equations and the corresponding ones is that the estimate now gives $y(x_0)$ in terms of $y(x_1)$ and not vice versa, and the change in the integration bounds from $(0, 1)$ to $(-1, 0)$.

1.2 $\delta_p(J)$ and $\delta_p^\star(J)$

In equation (12) of [6], the symbol $\gamma_{p,j}$ (written without a comma in the subscript by Pickard) is implicitly defined

$$\Delta^j f_{-j} = \sum_{p=0}^{j}\gamma_{p,j} f_{-p}$$

Thus powers of the difference operator are expanded in the tabular points of f. The coefficients of this expansion are the alternating binomial coefficients:

1 -1
1 -2 1
1 -3 3 -1
1 -4 6 -4 1

or equivalently,

$$\gamma_{p,j} = (-1)^p \binom{j}{p}$$

This allows terms of the form $\beta_j \Delta^j f_{-j}$ to be written $\sum_{p=0}^{j}\gamma_{p,j}\beta_j f_{-p}$. We then define

$$\alpha_p(J) = \sum_{j=p}^{J}\gamma_{p,j}\beta j$$

which, grouping the summation differently, allows us to further simplify the estimate for $y(x_1)$ given in Equation (4) as

$$y(x_1) = y(x_0) + h\sum_{p=0}^{J} \alpha_p(J) f_{-p} + E_J$$

Like β_j, $\alpha_p(J)$ are fractions with a denominator dividing $L(j)j!$. As before, it is convenient to multiply out by this denominator to get integers, here $\delta_p(J) = L(J)J!\alpha_p(J)$.

To relate $\delta_p(J)$ to $\aleph_j$, we have

$$\delta_p(J) = L(J)J!\sum_{j=p}^{J} \gamma_{p,j}\beta_j$$

and therefore

$$\delta_p(J) = \sum_{j=p}^{J} \frac{L(J)J!}{L(j)j!}\gamma_{p,j}\aleph_j$$

where all the terms on the right hand side, including the fraction, are integers. This, together with the values of $\aleph_j$ given by (1) and (2), allow us to calculate arbitrary values of $\delta_p(J)$.

An exactly analogous consideration exists for $\delta^\star_p(J)$.

The Python code [4] uses essentially the formulae given here to obtain terms of $\aleph_j$, $\delta_p(J)$, $\aleph^\star_j$, etc. That code contains explicit functions to calculate terms of all the encyclopedia sequences A002397-A002406, A260780 and A260781.

2 Concordance

Pickard cites both the books [1] and [5] as providing tables of the coefficients β_j and $\beta^\star_j$, albeit with fewer entries than his own.

The Collatz version is chapter 2, section 3 of [1], where he refers to the 'Adams interpolation method' and the 'Adams extrapolation method'. The Henrici version is chapter 5 of [5], where he refers to the methods as the Adams-Moulton and the Adams-Bashforth method.

Pickard [6]	Collatz [1]	Henrici [5]
β_j	β_j	γ_j
$\alpha_p(J)$	$\alpha_{J,p}$	$\beta_{J,p}$
$\beta^\star_j$	$\beta^\star_j$	$\gamma^\star_j$
$\alpha^\star_p(J)$	$\alpha^\star_{J,p}$	$\beta^\star_{J,p}$

Henrici gives a recursive formula for β_n in terms of β_i for i betwen 0 and $n-1$ on page 193. This potentially represents an easier way of obtaining terms of this sequence than (1).

3 Further notes

The paper [2], which we have not been able to get hold of, certainly defines a similar collection of coefficients. The sequence `https://oeis.`

org/A140825 and the paper [3] do not give us all the information we need to be sure of the exact relationship between those coefficients and those of Pickard.

References

[1] Lothar Collatz. *The Numerical Treatment of Differential Equations.* Springer Verlag, 3 edition, 1960. Retrieved from http://libgen.rs/book/index.php?md5=FDED4E8F79764E04ACBCEF80F0AC082D.

[2] P. Curtz. Intégration numérique des systèmes différentiels à conditions initiales, 1969. Cited in https://oeis.org/A140825.

[3] Philippe Flajolet, Xavier Gourdon, and Bruno Salvy. Sur une famille de polynômes issus de l'analyse numérique. *INRIA Rapport de recherche*, 1857, February 1993. https://hal.inria.fr/inria-00074815/document.

[4] Jack Grahl. A002405.py. https://github.com/jwg4/numerical/blob/main/A002402/A002405.py.

[5] Peter Henrici. *Discrete variable methods in ordinary differential equations.* Wiley, New York, 1962. Available to consult at https://archive.org/details/discretevariable0000henr/.

[6] William F. Pickard. Tables for the step-by-step integration of ordinary differential equations of the first order. *Journal of the Association for Computing Machinery*, 11(2):229–233, April 1964. https://oeis.org/A002397/a002397.pdf.