A Brief Survey of Extrapolation Quadrature[*]

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Since the dawn of mathematics, historians and others have found many isolated instances of extrapolation being used in numerical calculation. However, the first serious proponent seems to have been Richardson (1923). His technique, *aka* "the deferred approach to the limit," can be applied to the numerical evaluation of any quantity L, which can be defined as a limit as h approaches zero of an approximation $L(h)$ when this $L(h)$ has an expansion of the form

$$L(h) = L + a_1 h + a_2 h^2 + ... + a_r h^r + O(h^{r+1}). \qquad (1)$$

In other words, the discretization error $L(h) - L$ has a power series expansion in the parameter (usually a step length) h. Richardson suggested his technique particularly for large calculations. For example, L might be the solution at some point of a differential equation and $L(h)$ its approximation obtained by using a discrete analogue based on a finite step length h. Richardson's technique comprised evaluating several relatively poor approximations based on different moderate values if h, and then extrapolating these values to obtain an approximation for $L(0)$. This was proposed as an alternative to using a single, much smaller value of h. A strength of this approach is that numerical values of the coefficients a_i are not needed. We simply need to know that these coefficients exist.

During the subsequent 25 years, Richardson's approach was consistently ignored or misunderstood in environments where the analysis was available and, where in retrospect, the method would have been powerful. But, in the second half of the twentieth century, Richardson's idea was widely exploited in several numerical areas. Many expansions that can be used for extrapolation have been discovered, some of which are displayed below. In the discipline of numerical quadrature, this body of theory is sometimes referred to as *extrapolation quadrature.* This theory has several aspects. The first, dealt with in this talk, is the establishment of the expansion. But also of significant importance are questions relating to its use: in particular, selecting which values of h to use, organizing such a calculation, avoiding amplification of roundoff and other calculational error, and comparing other methods for handling the same problem.

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This talk was devoted exclusively to the first problem, the discovery of suitable asymptotic expansions on which to base the expansions and is restricted to numerical quadrature.

In 1955 this technique was applied somewhat diffidently by Romberg to the numerical integration of a $C^{(\infty)}$ integrand $f(x)$ over a finite interval $[0,1]$, using for $L(h)$ the $m = 1/h$ panel trapezoidal rule approximation, which we shall denote by $Q^{(m)}$. In this case, the expansion (1) turns out to be the classical Euler-Maclaurin asymptotic expansion

$$Q^{(m)} f - If = \sum B_j / m^j. \tag{2}$$

Romberg used a sequence of panel numbers $m = 1/h$ that were in geometric progression. During the next ten years, a systematic development of this simple theory took place. The Neville algorithm was used to carry out the extrapolation in an iterative manner. The tableau associated with this algorithm became known as the *Romberg T-table*. It transpired that $Q^{(m)}$ could be generalized to become the *m-copy* version of any quadrature rule Q. This gave an expansion that, depending on the nature of Q, might be even in character and might have other specified coefficients missing. One could use other sequences of panel numbers m and still form a Romberg table of extrapolants. Each element $T_{k,p}$ of this table is a somewhat involved linear sum of function values and so is, in its own right, the result of a different quadrature rule evaluation. Each is of specified algebraic and trigonometric degree. But, significantly, the expansion (2) could be regarded as a generator of quadrature rules.

The presentation included a short discussion about the circumstances under which the Euler-Maclaurin expansion converges and what happens when $f(x)$ is $C^{(\infty)}$ and periodic with period 1.

In the case when $f(\mathbf{x})$ is regular, the same theory has been applied in a multidimensional setting. The generalization to the hypercube $[0,1]^s$ is straightforward. The same generalization to the s-dimensional simplex (or even to the triangle) is quite difficult. At first, careful attention has to be paid to what is meant by $Q^{(m)}$. Several definitions are possible, but each produces a consistent mathematical theory. The resulting asymptotic expansion is of identical form to that of the hypercube. But, the coefficients have quite different representations. In cases where simple integral representations of the coefficients in the one-dimensional expansion (2) are known, these generalize readily to the hypercube, and not at all to the triangle or simplex.

In 1965, the one-dimensional theory was enriched by the discovery of a more general version of (2). This is usually attributed to Lyness and Ninham, but in fact Navot had discovered it several years previously.

Let $f(x) = x^{\alpha} g(x)$ with $g(x)$ regular, and let

$$Qf = \sum w_j f(x_j)$$

be any quadrature rule approximation to the exact integral

$$If = \int_0^1 f(x)dx,$$

this approximation being exact for constant f, that is, $\sum w_j = 1$; and let $Q^{(m)}f$ denote the m-copy version of Q. Then the following is an asymptotic expansion for the error functional

$$Q^{(m)}f - If = \sum_{j=1} A_{j+1+\alpha}/m^{(j+1+\alpha)} + \sum_{j=1} B_j/m^j, \tag{3}$$

where the coefficients A_j and B_j do not depend on m. There is a large literature about this sort of expansion. The result generalizes to negative α, the integral If being an HFP integral. When α is a negative integer, an additional term $K\mathrm{log}m$ is required in the expansion. A simple generalization of (3) is available for integrand functions that have algebraic singularities at both ends of the integration interval. And there are corresponding expansions for integrand functions having joint algebraic-logarithmic singularities (ones of the form $x^\alpha \log^n x$) at one or at both ends of the integration interval.

The next major development appeared in 1976. This extended Navot's result to integrand functions $f(\mathbf{x})$ having a singularity (of a specified type) at a vertex of the s-dimensional hypercube $[0,1]^s$ of integration. A homogeneous function $h(x)$ of degree α is one that satisfies $h(\lambda\mathbf{x}) = \lambda^\alpha h(\mathbf{x})$ for all $\lambda > 0$. The new result applied to $f(\mathbf{x}) = \mathbf{h}_\alpha(\mathbf{x})\mathbf{g}(\mathbf{x})$, where $h_\alpha(\mathbf{x})$ is a homogeneous function of degree α and has no singularity in the integration hypercube except at the origin; and, as usual, $g(\mathbf{x})$ is regular in this hypercube. For such a function,

$$Q^{(m)}f - If = \sum_{j=1}(A_{j+s+\alpha} + C_{j+s+\alpha}\mathrm{log}m)/m^{(j+s+\alpha)} + \sum_{j=1} B_j/m^j. \tag{4}$$

The coefficient $C_\lambda = 0$ unless λ is an integer. The function r^α and many others are homogeneous.

Subsequently, expansions were derived for many variants having joint algebraic logarithmic singularities at a vertex, and having different singularities, each being of this same general type, located at different vertices. The incorporation of line singularities located on an edge or face has proved difficult. At present, in two dimensions, there is a known expansion for an integrand having a "full corner singularity", that is

$$f(x,y) = x^\alpha y^\beta r^\rho g(x,y)$$

The corresponding theory for the simplex

$$\Delta : x_i \geq 0; i = 1,2,...s; \qquad \sum x_j \leq 1$$

can be derived geometrically from the corresponding results for the hypercube (with singularity) and the result for the simplex (with no singularity).

It is well known that when two regions are related by an affine transformation, a quadrature rule for the one region can be transformed to one for the other by using the same affine transformation. This is valid for quadrature rules with weight functions, but of course the weight function has to be transformed too. An implication is that a Gaussian rule for the triangle Δ above, with weight function $1/r$ at one vertex, would be basically different from any corresponding Gaussian rule for an equilateral triangle with the same weight function $1/r$ at a vertex. If one has available a set of weights and abscissas for one, they are irrelevant for the other. On the other hand, the affine transformation of a homogeneous function is another homogeneous function of the same degree. Thus, any extrapolation technique for one can be used immediately on the other. This circumstance does not seem to be widely known; but it provides a compelling reason for using extrapolation quadrature over polygonal regions of integrand functions having algebraic singularities at vertices.

Recent results include extensions to Jacobian-free integration over curved surfaces and to integrands involving the Laplacian operator. Results obtained by using Sidi transformations may be extrapolated. The numerical evaluation of Hadamard finite part integrals is being pursued by Monegato. And, currently, Verlinden is developing a new approach to constructing all the standard expansions within a single framework, based on the Mellin transform.

The talk finished with a numerical example in which the product mid-point rule was used very successfully to integrate the function $cos[arctan(x/y)]$ over the square $[0,1]^2$. This integrand is not Hölder continuous at the origin.
