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Monotonicity in Romberg Quadrature

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Abstract. Monotonicity of one or more derivatives of the integrand is shown to imply a corresponding property of the approximating Romberg scheme. This is of importance in connection with error estimation by majorants [6]. The monotonicity properties are derived from an elementary study of the kernel functions involved. A possible explanation is given of the monotonicity which frequently occurs in applications where nothing is presupposed about the signs of derivatives of the integrand. Finally, a nonlinear addition to Havie's scheme is suggested.

Following Bauer, Rutishauser, and Stiefel [1] (B.R.S.) and Håvie [2] we denote by $T_0^{(k)}$ and $U_0^{(k)}$ the approximations to $\int_0^1 f(x)\,dx$ by the trapezoidal and the rectangular rules with step sizes 2^{-k}, $k = 0, 1, \cdots$. Repeated Richardson extrapolation leads to the ordinary and modified Romberg schemes $T_m^{(k)}$ and $U_m^{(k)}$ satisfying

$$T_m^{(k)} = T_{m-1}^{(k+1)} + (T_{m-1}^{(k+1)} - T_{m-1}^{(k)})/(4^m - 1), \tag{1}$$

$$U_m^{(k)} = 2T_m^{(k+1)} - T_m^{(k)}. \tag{2}$$

We may form an aggregate table illustrated in Fig. 1.

$$\begin{array}{llll}
T_0^{(0)} & & & \\
T_0^{(1)} & T_1^{(0)} \ddots & & \\
T_0^{(2)} & T_1^{(1)} & \ddots & \\
\vdots & & T_{p-1}^{(0)} & \\
T_0^{(p)} & \cdots\cdots & T_{p-1}^{(1)} & T_p^{(0)} \\
U_0^{(p-1)} & \cdots\cdots & U_{p-1}^{(0)} & \\
\vdots & & \cdot^{\cdot^{\cdot}} & \\
U_0^{(1)} & & & \\
U_0^{(0)} & & &
\end{array}$$

FIGURE 1

Håvie [2] suggested the approximation of $\int_0^1 f(x)\,dx$ by $\frac{1}{2}(T_m^{(k)} + U_m^{(k-1)})$ with the error estimate $\frac{1}{2}\,|T_m^{(k)} - U_m^{(k-1)}|$. Ström [5] proved this inclusion to be strict if $f^{(2m+2)}(x)$ is of definite sign in (0, 1) and extended this restricted result to "majorizable" functions. In essence, f is "majorizable" if F is known such that $(F \pm f)^{(2m+2)}(x)$ both

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are of (the same) definite sign in (0, 1) (Ström [6]). Then the inclusion is again valid if the *error estimate* is computed from the table associated with $\int_0^1 F(x)\,dx$. It is hence of interest to know how a monotonicity property such as $f^{(2m+2)}(x) \geqq 0$ propagates to the Romberg tables. In a number of practical cases, where $f^{(2m+2)}(x)$ in general is not of definite sign, monotonicity has, nevertheless, been observed in the Romberg schemes. The reasons for this will also become apparent. Finally, it is of general interest to approximate $U_p^{(0)}$, the missing "partner" of $T_p^{(0)}$.

Definition 1. A function Φ is of class E ("Even") if

(i) $\Phi(x)$ is nonnegative in (0, 1) and nondecreasing in $(0, \frac{1}{2})$,

(ii) $\Phi(0) = \Phi(1) = 0$,

(iii) $\Phi(x) = \Phi(1 - x)$,

(iv) $\Phi(x) = \Phi(x + 1)$.

This notation was borrowed from Lyness [4].

Definition 2. Let ψ_1 be a given function, $\psi_1(x + 1) = \psi_1(x)$. Furthermore, let $\kappa_k = 1/(4^{k-1} - 1)$, $k = 2, 3, \cdots$, and define $\psi_2, \psi_3 \cdots$, through

$$\begin{aligned} \psi_k'' &= \kappa_k(\psi_{k-1}(2x) - \psi_{k-1}(x)), \\ \psi_k(0) &= \psi_k(1) = 0. \end{aligned} \tag{3}$$

The sequence $\psi_1, \psi_2, \cdots$, denoted by $\boldsymbol{\psi}_1$, will be called a R(omberg)-sequence (generated by ψ_1). Note that each ψ_k has period 1 and that $\psi_k'(0) = 0$ for $k \geqq 2$. An R-sequence with all its members of class E is called an ER-sequence.

An argument by B.R.S. may be stated as a useful lemma.

LEMMA 1. *An R-sequence generated by a function of class E is an ER-sequence.*

This lemma is fundamental to the subsequent results. If the first member of an ER-sequence is nonnegative, so are all subsequent members.

We also need a more obvious result for later reference.

LEMMA 2. *Any finite linear combination of R-sequences is an R-sequence. If* $\{\psi_i(x)\}_{i=1}$ *form an R-sequence and q is a nonnegative integer, then* $\{4^{-(k-1)q}\psi_k(2^q x)\}_{k=1}$ *form an R-sequence.*

Now

$$\begin{aligned} T_m^{(k)} &\qquad + 4^{-(m+1)k} \int_0^1 b_{m+1}(2^k x) f^{(2m+2)}(x)\,dx \\ &= \int_0^1 f(x)\,dx \\ U_m^{(k-1)} &\qquad - 4^{-(m+1)(k-1)} \int_0^1 c_{m+1}(2^{k-1}x) f^{(2m-2)}(x)\,dx \end{aligned} \tag{4}$$

where $\mathbf{b}_1$ is an ER-sequence (B.R.S.). Hence relation (2) and Lemma 2 imply that $\mathbf{c}_1$ is an R-sequence and, since $b_1(x) = x(1 - x)/2$, $0 \leqq x \leqq 1$, it follows that

$$\begin{aligned} c_1(x) &= x^2/2, & 0 \leqq x \leqq \tfrac{1}{2}, \\ &= (1 - x)^2/2, & \tfrac{1}{2} \leqq x \leqq 1, \end{aligned}$$

and also, through Lemma 1, that $\mathbf{c}_1$ is an ER-sequence (Ström [5]). Håvie [3] discusses $\mathbf{b}_1$ and $\mathbf{c}_1$ extensively. Now let

$$\nabla T_m^{(k)} = T_m^{(k)} - T_m^{(k-1)},$$
$$\nabla U_m^{(k)} = U_m^{(k)} - U_m^{(k-1)}. \tag{5}$$

Then our first results may easily be summarized.

THEOREM 1. *Let* $f^{(2m+2)}(x) \geqq 0$. *Then*

(i) $\nabla T_m^{(k)} \leqq 0$,
(ii) $\nabla U_m^{(k)} \geqq 0$,
(iii) $T_{m+1}^{(k-1)} \leqq T_m^{(k)}$,
(iv) $U_{m+1}^{(k-1)} \geqq U_m^{(k)}$,
(v) $\nabla T_m^{(k+1)}/\nabla T_m^{(k)} \leqq \frac{1}{2}$.

If, in addition, $f^{(2m+4)}(x) \geqq 0$, *then*

(vi) $1/4^{m+1} \leqq \nabla T_m^{(k+1)}/\nabla T_m^{(k)}$.

Before we outline a proof we note that if *all* the even derivatives of the integrand are nonnegative (e.g., the integrand is an absolutely or completely monotonic function) then there is monotonicity column-wise ((i) and (ii)) and row-wise ((iii) and (iv)) in the scheme. Hence the best error approximation with absolutely monotonic majorants (Ström [5], [6]) appears from a "complete" extrapolation. Also the results (i)–(v) of Theorem 1, being "asymptotically true" in very general cases, in practice often hold for very moderate values of k.

Proof of Theorem 1. First note that once (i) and (ii) have been established the other propositions follow as simple algebraic consequences of formulas (1), (2) and (5). The details are omitted. As $\nabla T_m^{(k)} = U_m^{(k-1)} - T_m^{(k)}$, (i) is an immediate consequence of (4) and the fact that $\mathbf{b}_1$ and $\mathbf{c}_1$ are *ER*-sequences. To prove (ii) we note that $\nabla U_m^{(k-1)}$ by definition is a linear combination of $T_m^{(k)}$'s and hence that its kernel functions form an *R*-sequence (Lemma 2). We find immediately that

$$\nabla U_m^{(k-1)} = 4^{-(k-2)(m+1)} \int_0^1 d_{m+1}(2^{k-2}x) f^{(2m+2)}(x)\, dx$$

where

$$d_{m+1}(x) = 2 \cdot 16^{-(m+1)} b_{m+1}(4x) - 4^{-(m+1)} \cdot 3 \cdot b_{m+1}(2x) + b_{m+1}(x).$$

In particular,

$$\begin{aligned} d_1(x) &= 0, & x &\in (0, \tfrac{1}{4}), \\ &= \tfrac{1}{8}(4x - 1), & x &\in (\tfrac{1}{4}, \tfrac{1}{2}). \end{aligned}$$

This together with the fact that b_1 is of class E shows that d_1 is of class E and hence that $\mathbf{d}_1$ is an *ER*-sequence (Lemma 1). This proves (ii). The definite signs of all occurring kernels also indicates that results like (i)–(v) are to be expected asymptotically in k if only $f^{(2m+1)}(1) \neq f^{(2m+1)}(0)$. Q.E.D.

Turning again to Fig. 1 we note that there is no natural "partner" of $T_p^{(0)}$ which, however, often is the best approximation. Let, in general,

$$\beta_m^{(k-1)} = \nabla U_m^{(k-1)}/\nabla U_m^{(k-2)} \quad \text{and} \quad \alpha_m^{(k)} = \nabla T_m^{(k)}/\nabla T_m^{(k-1)}.$$

If we know $\nabla U_m^{(k-1)}$ we may often approximate $U_m^{(k)}$ by the formula

$$\nabla U_m^{(k)} \approx \alpha_m^{(k)} \nabla U_m^{(k-1)}. \tag{6}$$

This follows from the relation

$$\beta_m^{(k)} = \alpha_m^{(k)}(1 - 2\alpha_m^{(k+1)})/(1 - 2\alpha_m^{(k)}),$$

where, in general, $\alpha_m^{(k)}$ and $\alpha_m^{(k+1)}$ are small ($\sim 1/4^{m+1}$) or at least approximately equal. (Compare also Theorem 1, props. (v) and (vi).) From (6) we thus find

$$U_m^{(k)} \approx \tilde{U}_m^{(k)} = U_m^{(k-1)} + \frac{\nabla T_m^{(k)}}{\nabla T_m^{(k-1)}} \nabla U_m^{(k-1)}. \tag{7}$$

If $\tilde{U}_m^{(k)}$ is added to a column and then used for further extrapolations just as $U_m^{(k)}$ would have been, we find an approximation to the missing element $U_p^{(0)}$. Fig. 2 illustrates this; the arrows and * indicate the additional extrapolations and elements.

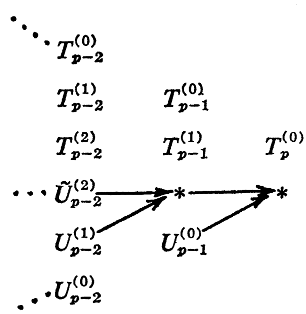

FIGURE 2

The rule was tried on a few examples and was successful when Håvie's method was. The error committed is generally very small. One may ask when the rule is correct in a strict sense. In a case where $f^{(2m+2)}(x) \geqq 0$ we infer from Theorem 1 (ii) that

$$U_m^{(k-1)} < \tilde{U}_m^{(k)} \leqq U_m^{(k)}$$

would imply that $\tilde{U}_m^{(k)}$ is a completely correct substitute for $U_m^{(k)}$ in the sense of the inclusion of $\int_0^1 f(x)\,dx$. This is equivalent to $\alpha_m^{(k+1)} \leqq \alpha_m^{(k)}$ which may be shown to hold asymptotically.

THEOREM 2. *If $f^{(i)}(1) > f^{(i)}(0)$ for $i = 2m+1, 2m+3$, then, for k sufficiently large,*

$$\nabla T_m^{(k+1)} \nabla T_m^{(k-1)} \leqq (\nabla T_m^{(k)})^2.$$

Proof. The Euler-Maclaurin expansion states that

$$T_m^{(k)} = \int_0^1 f(x)\,dx + \sum_{i=m+1}^{N} a_i^{(m)} 4^{-ik} + o(4^{-Nk}), \tag{8}$$

where

$$a_i^{(m)} = a_i^{(m-1)}(4^{m-i} - 1)/(4^m - 1),$$

$$a_i^{(0)} = (-1)^{i+1} \frac{|B_{2i}|}{(2i)!} (f^{(2i-1)}(1) - f^{(2i-1)}(0)),$$

B_{2i} are Bernoulli numbers. Hence

$$\operatorname{sign} a_i^{(m)} = (-1)^{m+i+1} \operatorname{sign}(f^{(2i-1)}(1) - f^{(2i-1)}(0)),$$

i.e. in particular

$$\operatorname{sign} a_{m+2}^{(m)} = -\operatorname{sign} a_{m+1}^{(m)} = -1. \tag{9}$$

From (8) follows

$$\nabla T_m^{(k)} = \sum_{i=m+1}^{N} a_i^{(m)} 4^{-ik}(1 - 4^i) + o(4^{-Nk}). \tag{10}$$

We now define

$$\Phi_k(t) = t^2 \nabla T_m^{(k+1)} - 2t \nabla T_m^{(k)} + \nabla T_m^{(k-1)}.$$

For k sufficiently large, the first term in (10) predominates. Hence, in view of (9),

$$\Phi_k(0) = \nabla T_m^{(k-1)} \leqq 0. \tag{11}$$

Also

$$\Phi_k(4^{m+1}) = \sum_{i=m+2}^{N} a_i^{(m)} 4^{-ik}(1 - 4^i)4^{-i} + o(4^{-Nk}).$$

Hence for k sufficiently large, sign $\Phi_k(4^{m+1}) = -$ sign $a_{m+2}^{(m)} = 1$ by (9), i.e. $\Phi_k(4^{m+1}) > 0$. This, together with (11), proves that $\Phi_k(t) = 0$ has two real roots for k sufficiently large showing that its discriminant must be nonnegative which precisely gives the required relation. Q.E.D.

Unfortunately the nonlinearity prevents the rule from being used in a strict majorant application and it is thus only proposed as a complement to Håvie's method.

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1. F. L. Bauer, H. Rutishauser & E. Stiefel, *New Aspects in Numerical Quadrature*, Proc. Sympos. Appl. Math., vol. 15, Amer. Math. Soc., Providence, R.I., 1963, pp. 198–218. MR **30** #4384.

2. T. Håvie, "On a modification of Romberg's algorithm," *Nordisk Tidskr. Informationsbehandling*, v. 6, 1966, pp. 24–30. MR **33** #3460.

3. T. Håvie, "Derivation of explicit expressions for the error terms in the ordinary and the modified Romberg algorithms," *Nordisk Tidskr. Informationsbehandling*, v. 9, 1969, pp. 18–29. MR **40** #5126.

4. J. N. Lyness & L. M. Delves, "On numerical contour integration round a closed contour," *Math. Comp.*, v. 21, 1967, pp. 561–577. MR **37** #4962.

5. T. Ström, "Strict error bounds in Romberg quadrature," *Nordisk Tidskr. Informationsbehandling*, v. 7, 1967, pp. 314–321. MR **36** #7329.

6. T. Ström, *Absolutely Monotonic Majorants and Their Use for Automatic Strict Error Estimation in Some Areas of Numerical Analysis*, Report NA 71.34, Department of Computer Science, Royal Institute of Technology, S-100 44 Stockholm, Sweden.