MONOTONICITY OF QUADRATURE APPROXIMATIONS

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ABSTRACT. For the general quadrature rules of Newton-Cotes we show that the convergence is monotone for the appropriate class of functions. Included are the well-known trapezoidal and Simpson rules.

Some time ago Szegő and Turán [3] showed that the Riemann sums $n^{-1} \sum_{i=1}^n f(i/n)$ form a nonincreasing sequence for any $f(x)$ which is increasing and concave. Recently Rivlin and I found that the trapezoidal sums $(f(0)+f(1))/2n + n^{-1} \sum_{i=1}^{n-1} f(i/n)$ also form a nonincreasing sequence, this time for $f(x)$ satisfying $f''(x) \geq 0$, $f'''(x) \leq 0$, $f \in C^3$. An analogous result was obtained by Molluzo [2] for the "Simpson rule" where the appropriate condition turned out to be $f^{iv}(x) \geq 0$, $f^v(x) \leq 0$, $f \in C^5$.

In each case the theme seems to be that the proper signum for the first two derivatives that "count" is sufficient for monotonicity. Thus in the trapezoidal case, since the rule is exact for linear functions, the first derivatives' size does not count. Similarly Simpson's rule is exact for cubics and so there the first three derivatives do not count. [Molluzo also set up the machinery to verify the monotonicity for the so-called $\frac{3}{8}$ -rule but the computations became unwieldy.]

The purpose of this note is to prove that this behavior does indeed persist for all of the Newton-Cotes rules. For reasons of brevity we will say "up" and "down" respectively to mean *nondecreasing* and *nonincreasing* and also we will say "plus" and "minus" to mean *nonnegative* and *nonpositive*.

LEMMA 1. Let $\mu(x)$ be a normalized BV function on $[0, 1]$ with $\mu(0)=0$ and let $\alpha \geq 0$. The necessary and sufficient condition (nasc) that

$$n^{-\alpha} \int_0^1 F\left(\frac{x}{n}\right) + F\left(\frac{x+1}{n}\right) + F\left(\frac{x+n-1}{n}\right) d\mu(x)$$

be a down sequence for every plus, down function, $F(x)$, is that both $x^{-\alpha}\mu(x)$ and $\mu(x) - \alpha x\mu(1)$ be down on $[0, 1]$

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PROOF. If we extend $\mu(x)$ to the whole positive line by the relation $\mu(x+1)=\mu(x)+\mu(1)$ then we have identically,

$$\int_0^1 F\left(\frac{x}{n}\right) + F\left(\frac{x+1}{n}\right) + \cdots + F\left(\frac{x+n-1}{n}\right) d\mu(x) = \int_0^1 F(x) d\mu(nx).$$

Integrating by parts we find this is, in turn, equal to

$$\mu(n)F(1) - \int_0^1 \mu(nx) dF(x).$$

We desire therefore, that

$$n^{-\alpha}\mu(n)F(1) - \int_0^1 (nx)^{-\alpha}\mu(nx)x^{\alpha} dF(x)$$

be a down sequence for every plus, down $F(x)$ and an obviously sufficient condition is that for each fixed $x \in (0, 1]$, $(nx)^{-\alpha}\mu(nx)$ be a down sequence. Furthermore choosing $F(x)$ as a simple jump function shows this condition to also be a necessary one.

Next we observe that if $t^{-\alpha}\mu(t)$ were a down function on $(0, \infty)$ this would surely insure the down nature of the sequence $(nx)^{-\alpha}\mu(nx)$. Conversely by choosing a small x and large values of n we can show that monotonicity of the sequences implies monotonicity of the function.

Thus far, then, our nasc is simply that $t^{-\alpha}\mu(t)$ be down on $(0, \infty)$ and we proceed to interpret this as a condition on $[0, 1]$.

For K any plus integer we have then that $(x+K)^{-\alpha}[\mu(x)+K\mu(1)]$ is down in $[0, 1]$. We may differentiate this expression and obtain, in the language of measures, that

$$(x+K)^{-\alpha} d\mu(x) - \alpha(x+K)^{-\alpha-1}[\mu(x) + K\mu(1)] dx \leq 0$$

or

$$(x d\mu(x) - \alpha\mu(x) dx) + K(d\mu(x) - \alpha\mu(1) dx) \leq 0.$$

This holding for all plus integers K , finally, is equivalent to both

$$x d\mu(x) - \alpha\mu(x) dx \leq 0, \quad d\mu(x) - \alpha\mu(1) dx \leq 0$$

and our proof is complete.

An important case for us will be that of "symmetric" $\mu(x)$, i.e., those for which $\mu(1-x)=\mu(1)-\mu(x)$. In that case the second of our conditions is a consequence of the first. Namely if $x d\mu(x) \leq \alpha\mu(x) dx$ then

$$\begin{aligned} (1-x) d\mu(x) &= -(1-x) d\mu(1-x) \leq \alpha\mu(1-x) dx \\ &= \alpha\mu(1) dx - \alpha\mu(x) dx \end{aligned}$$

and adding gives $d\mu(x) \leq \alpha\mu(1) dx$. Thus we have the

COROLLARY. For symmetric $\mu(x)$ (with $\mu(0)=0$) the nase that

$$n^{-\alpha} \int_0^1 F\left(\frac{x}{n}\right) + \cdots + F\left(\frac{x+n-1}{n}\right) d\mu(x)$$

be down for all plus, down $F(x)$ is that $x^{-\alpha}\mu(x)$ be down on $(0, 1]$.

We now introduce the Newton-Cotes rules. So let N be a positive odd integer. For $f(x)$ any continuous function on $[0, 1]$ we denote by $A(x)$ the N th degree polynomial interpolating $f(x)$ at $0, 1/N, 2/N, \dots, N/N$ and $B(x)$ the $(N-1)$ th degree polynomial interpolating $f(x)$ at $0, 1/(N-1), 2/(N-1), \dots, (N-1)/(N-1)$. The Newton-Cotes functionals of first and second kinds are given respectively by

$$L^{(1)}(f(x)) = \int_0^1 A(x) dx, \quad L^{(2)}(f(x)) = \int_0^1 B(x) dx$$

and the Newton-Cotes rules are then given by

$$L_n(f(x)) = \frac{1}{n} L\left(f\left(\frac{x}{n}\right) + f\left(\frac{x+1}{n}\right) + \cdots + f\left(\frac{x+n-1}{n}\right)\right),$$

$$L = L^{(1)}, \quad L^{(2)}.$$

For example the trapezoidal rule familiarly written as

$$\frac{f(0) + 2f(1/n) + 2f(2/n) + \cdots + f(1)}{2n}$$

emerges as $L_n^{(1)}(f(x))$ for $N=1$. Similarly Simpson's rule

$$\frac{f(0) + 4f(1/2n) + 2f(2/2n) + \cdots + 4f((2n-1)/2n) + f(1)}{6n}$$

is simply $L_n^{(2)}(f(x))$ when $N=3$.

In this context we state our general

THEOREM. If $f(x) \in C^{N+2}$, $f^{(N+1)}(x) \geq 0$, $f^{(N+2)}(x) \leq 0$ on $[0, 1]$ then $L_n(f(x))$ is a down sequence ($L=L^{(1)}$ or $L^{(2)}$).

PROOF. It is well known that for $f(x)$ a polynomial of degree N the rules are exact, i.e., that $L^{(1)}(f(x))=L^{(2)}(f(x))=\int_0^1 f(x) dx$. This says that $\int_0^1 A(x) dx = \int_0^1 f(x) dx$ and $\int_0^1 B(x) dx = \int_0^1 f(x) dx$ and the first of these is trivial since $A(x) \equiv f(x)$. The second relation follows from the observations that $f(x)-B(x)$ is a constant multiple of

$$\prod_{j=0}^{N-1} (x - j/(N-1))$$

and $\int_0^1 \prod_{j=0}^{N-1} (x - j/(N-1)) dx = 0$ since $\prod_{j=0}^{N-1} (1-x) \equiv -\prod_{j=0}^{N-1} (x - j/(N-1))$.

² Sending x into $1-x$ allows us to replace these conditions, if we wish, by $f^{(N+1)}(x) \geq 0$, $f^{(N+2)}(x) \geq 0$.

Thus $L(f(x)) - \int_0^1 f(x) dx$ annihilates all polynomials of degree N and as such is a (bounded) linear functional of $f^{(N+1)}(x)$ alone. Write $F(x) = f^{(N+1)}(x)$ and conclude that $L(f(x)) - \int_0^1 f(x) dx = \int_0^1 F(x) d\mu(x)$ so that

$$\begin{aligned} L_n(f(x)) - \int_0^1 f(x) dx \\ = n^{-(N+2)} \int_0^1 F\left(\frac{x}{n}\right) + F\left(\frac{x+1}{n}\right) + \cdots + F\left(\frac{x+n-1}{n}\right) d\mu(x) \end{aligned}$$

and we find ourselves in the exact situation described by our Lemma. Indeed it is a simple observation that our $\mu(x)$ is symmetric and we may even avail ourselves of the Corollary to that Lemma. To prove our theorem, then, we need only check that $t^{-(N+2)}\mu(t)$ is down on $[0, 1]$ and we prove in fact that $t^{-(N+1)}\mu(t)$ is.

We now derive a formula for $\mu(t)$ implicit in the standard results on the Newton-Cotes rules (see [1]). The approach we use, however, is self-contained and avoids lengthy discussion in the calculus of finite differences.

For convenience in the forthcoming calculation let us expand the underlying interval from $[0, 1]$ and redefine

$$L^{(1)}(f(x)) = \int_0^N A(x) dx = \int_0^N f^{(N+1)}(x) d\mu^{(1)}(x) + \int_0^N f(x) dx$$

(where $A(x)$ is the interpolating polynomial to $f(x)$ at $0, 1, 2, \dots, N$):

$$L^{(2)}(f(x)) = \int_0^{N-1} B(x) dx = \int_0^{N-1} f^{(N+1)}(x) d\mu^{(2)}(x) + \int_0^{N-1} f(x) dx$$

(where $B(x)$ is the interpolating polynomial to $f(x)$ at $0, 1, 2, \dots, N-1$).

In this new normalization we now write $dv(x) = d\mu^{(1)}(x) - d\mu^{(2)}(x)$ and we will prove the monotonicity of $x^{-(N+1)}\mu^{(2)}(x)$ and $x^{-(N+1)}v(x)$ which is more than sufficient. If indeed we note that $A(x) - B(x)$ is a constant multiple of $x(x-1) \cdots (x-N+1)$ then we obtain

$$\int_0^{N-1} (A(x) - B(x)) dx = C \int_0^{N-1} x(x-1) \cdots (x-N+1) dx = 0$$

and we conclude that

$$L^{(1)}(f(x)) - L^{(2)}(f(x)) = \int_{N-1}^N A(x) dx$$

so that

$$(1) \quad \int_0^N f^{(N+1)}(x) dv(x) = \int_{N-1}^N (A(x) - f(x)) dx$$

and of course we also have

$$(2) \quad \int_0^{N-1} f^{(N+1)}(x) d\mu(x) = \int_0^{N-1} (B(x) - f(x)) dx.$$

Now set $f(x) = e^{-\lambda x}$. By Lagrange's interpolation formula we have

$$A(x) = \frac{x(x-1)\cdots(x-N)}{[N]} \sum_{j=0}^N (-1)^j \binom{N}{j} \frac{e^{-j\lambda}}{j-x},$$

$$B(x) = \frac{-x(x-1)\cdots(x-N+1)}{[N-1]} \sum_{j=0}^{N-1} (-1)^j \binom{N-1}{j} \frac{e^{-j\lambda}}{j-x},$$

also, setting $\lambda=0$, e.g., we obtain

$$1 = \frac{x(x-1)\cdots(x-N)}{[N]} \sum_{j=0}^N (-1)^j \binom{N}{j} \frac{1}{j-x},$$

$$1 = - \frac{x(x-1)\cdots(x-N+1)}{[N-1]} \sum_{j=0}^{N-1} (-1)^j \binom{N-1}{j} \frac{1}{j-x},$$

so that, by subtraction,

$$A(x) - f(x) = \frac{x(x-1)\cdots(x-N)}{[N]} \sum_{j=0}^N (-1)^j \binom{N}{j} \frac{e^{-j\lambda} - e^{-x\lambda}}{j-x},$$

$$B(x) - f(x) = - \frac{x(x-1)\cdots(x-N+1)}{[N-1]} \sum_{j=0}^{N-1} (-1)^j \binom{N-1}{j} \frac{e^{-j\lambda} - e^{-x\lambda}}{j-x}.$$

Next note that $(e^{-\lambda j} - e^{-\lambda x})/(j-x) = \lambda \int_0^1 e^{-\lambda xs} e^{-\lambda j(1-s)} ds$ so that the above formulas become

$$(3) \quad A(x) - f(x) = \frac{-x(x-1)\cdots(x-N)}{[N]} \lambda \int_0^1 e^{-\lambda xs} (1 - e^{-\lambda(1-s)})^N ds,$$

$$(4) \quad B(x) - f(x) = \frac{x(x-1)\cdots(x-N+1)}{[N-1]} \lambda \int_0^1 e^{-\lambda xs} (1 - e^{-\lambda(1-s)})^{N-1} ds.$$

We now abbreviate these by writing

$$P(x) = - \frac{x(x-1)\cdots(x-N)}{[N]},$$

$$(5) \quad Q'(x) = \frac{x(x-1)\cdots(x-N+1)}{[N-1]}, \quad Q(0) = 0$$

and we observe the trivial facts that $P(x) \geq 0$ in $[N-1, N]$ and $Q(N-1) = 0$, and also the somewhat less trivial fact that $Q(x) \geq 0$ on $[0, N-1]$. A

simple proof can be given by induction. Since $(t-N+2)(t-N+1)$ is plus, down in $[0, N-3]$ we have, for x in this interval,

$$\int_0^x t(t-1)\cdots(t-N+1)dt = (N-1)(N-2)\int_0^x t(t-1)\cdots(t-N+3)dt$$

and the latter is ≥ 0 by the inductive hypothesis. For $x \in [N-3, N-1]$, on the other hand, we simply use $Q(N-1-x) = Q(x)$.

Comparing (3) and (4) then with (1) and (2) gives

$$(6) \quad \int_0^N e^{-\lambda x} dv(x) = \int_{N-1}^N P(x) \int_0^1 e^{-\lambda xs} \left(\frac{1 - e^{-\lambda(1-s)}}{\lambda} \right)^N dt dx,$$

$$(7) \quad \int_0^{N-1} e^{-\lambda x} d\mu(x) = \int_0^{N-1} Q(x) \int_0^1 e^{-\lambda xs} \left(\frac{1 - e^{-\lambda(1-s)}}{\lambda} \right)^{N-1} s ds dx,$$

where in the latter we have integrated by parts.

If we now write $(1 - e^{-\lambda(1-s)})/\lambda = \int_0^{1-s} e^{-\lambda u} du$ so that

$$\left(\frac{1 - e^{-\lambda(1-s)}}{\lambda} \right)^K = \int_0^{1-s} \cdots \int_0^{1-s} \exp\{-\lambda(u_1 + u_2 + \cdots + u_k)\} du_1 \cdots du_k,$$

we can replace (6) and (7) by

$$(8) \quad \begin{aligned} & \int_0^N e^{-\lambda x} dv(x) \\ &= \int_{N-1}^N P(x) \int \cdots \int_{\mathcal{H}} e^{-\lambda(xs + u_1 + u_2 + \cdots + u_N)} du_1 du_2 \cdots du_N ds dx \end{aligned}$$

where $\mathcal{H}$ is defined by $u_i \geq 0$, $s \geq 0$, $u_i + s \leq 1$,

$$(9) \quad \begin{aligned} & \int_0^{N-1} e^{-\lambda x} d\mu(x) \\ &= \int_0^{N-1} Q(x) \int \cdots \int_{\mathcal{H}'} e^{-\lambda(xs + u_1 + \cdots + u_{N-1})} du_1 \cdots du_{N-1} ds dx. \end{aligned}$$

We can now identify $v(t)$ and $\mu(t)$ since these equalities hold for all λ . We have namely

$$\begin{aligned} v(t) &= \int_{N-1}^N P(x) \int_{\substack{u_i \geq 0, s \geq 0; u_i + s \leq 1; xs + u_1 + \cdots + u_N \leq t}} \cdots \int du_1 du_2 \cdots du_N ds dx, \\ \mu(t) &= \int_0^{N-1} Q(x) \int_{\substack{u_i \geq 0, s \geq 0; u_i + s \leq 1; xs + u_1 + \cdots + u_{N-1} \leq t}} \cdots \int s du_1 \cdots du_{N-1} ds dx \end{aligned}$$

changing variables by $u_i = tU_i$, $s = tS$ we obtain finally

$$\frac{v(t)}{t^{N+1}} = \int_{N-1}^N P(x) \int_{U_i \geq 0, S \geq 0: U_i + S \leq 1/t: xS + U_1 + \dots + U_{N-1} \leq 1} \dots \int dU_1 \dots dU_{N-1} dS dx,$$

$$\frac{\mu(t)}{t^{N+1}} = \int_0^{N-1} Q(x) \times \int_{U_i \geq 0, S \geq 0: U_i + S \leq 1/t: xS + U_1 + \dots + U_{N-1} \leq 1} S dU_1 dU_2 \dots dU_{N-1} dS dx.$$

The inner integrals are clearly down as functions of t and so the proof is complete.

Since we had the luck to prove that $t^{-(N+1)}\mu(t)$ is down, rather than only that $t^{-(N+2)}\mu(t)$ is, it seems we should be able to conclude more monotonicity than that of L_n . Indeed this is the case and in fact we find that we have proved

THEOREM'. If $f(x) \in C^{N+2}$, $f^{(N+1)}(x) \geq 0$, $f^{(N+2)}(x) \leq 0$ on $[0, 1]$ then $nL_n(f(x)) - n \int_0^1 f(x) dx$ is down ($L = L^{(1)}$ or $L^{(2)}$).

In particular applying this to the trapezoidal rule gives the interesting

COROLLARY. For $f(x) \in C^3$, $f''(x) \geq 0$, $f''' \leq 0$ on $[0, 1]$ we have

$$\sum_{j=1}^n f\left(\frac{j}{n+1}\right) - \sum_{j=1}^{n-1} f\left(\frac{j}{n}\right) \leq \int_0^1 f(x) dx.$$

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