Progress in the Bayesian Automatic Adaptive Quadrature

Gh. Adam, S. Adam

e-mail: adamg@jinr.ru, Laboratory of Information Technologies, JINR, Dubna

DFT IFIN-HH, Magurele – Bucharest, 077125, Romania

Progress obtained under the addition of Bayesian inference to the automatic adaptive quadrature scheme developed in `QUADPACK` [1] was recently discussed in [2]. The Bayesian inference involves a set of necessary consistency criteria allowing the identification of the spurious local quadrature rule (q, e) outputs *prior to their activation.* This is found to increase significantly the output reliability under the lack of *a priori* knowledge on the behaviour of the integrand over the integration domain.

We search for the numerical solution by automatic adaptive quadrature [1]–[4] of a (proper or improper) one-dimensional Riemann integral,

$$I \equiv I[a, b]f = \int_a^b f(x)dx \ , \qquad (1)$$

where the integrand function $f : [a, b] \to \mathbf{R}$ is assumed to be continuous almost everywhere on $[a, b]$, such that (1) exists and is finite.

There are integrand features which result in conspicuously unreliable local quadrature rule (q, e) outputs if properly questioned and identified:

– Occurrence of a range of variation of a monotonic integrand which exceeds the worst case bound inferred from the polynomial set spanning the interpolatory quadrature sum.

– Inconsistent slope integrand approximations at the subrange ends.

– Integrand oscillations at a rate of variation beyond the current quadrature knot set resolving power (too near to each other neighbouring extrema or too many integrand extrema over a given subrange).

– Isolated irregular integrand extremum.

– Occurrence of a finite jump with finite lateral derivatives, immersed into a monotonicity subrange of the integrand.

– Same as previous, but turning point.

– Severe precision loss due to cancellation by subtraction.

The specific decisions following from the identification of one or another of the abovementioned cases depends on the diagnostic. There are three possible continuations:

(i) *Stop immediately the computation* and return the appropriate error flag (when there is no hope to improve the output for the present problem formulation).

(ii) Proceed *immediately* to *symmetric subrange bisection* (when it is expected that the refinement of the discretization into subranges will result into a better resolved integrand profile).

(iii) Proceed *immediately* to the solution of a number of auxiliary problems.

If the occurrence of an *inner* isolated offending point x_s was inferred, then resolve its location inside (α, β) *to machine accuracy.*

Proceed then to the splitting $[\alpha, \beta] = [(\alpha, x_s) \cup (x_s, \beta)]$. The abscissa x_s will be *locked* from now on at subrange boundaries within the subrange subdivision process of $[a, b]$. If $x_s = a$ or $x_s = b$, then solve *one lateral boundary layer problem* [5, 6], at x_s^+ or x_s^- respectively, in order to determine the *nature* of the integrand behaviour at x_s as well as appropriate integrand lateral limits. If $x_s \in (a, b)$, then solve *two lateral boundary layer problems*, at x_s^- and x_s^+ respectively.

The solutions of the auxiliary problems define the further continuation of the algorithm.

If x_s is an essential singular point (i.e., it associates a singularity of $f(x_s)$ together with infinitely many oscillations of $f(x)$ in its neighbourhood (like, e.g., $\sin(1/x)$ at $x = 0^+$)), then further continuation is useless. The computation is *stopped immediately* and the appropriate error flag is returned.

If x_s corresponds either to a finite jump or a turning point with finite lateral derivative, then its contribution to the original Riemann integral is nil. The local quadrature outputs (q, e) *become insensitive* to the occurrence of the nearby offending locked endpoint.

If there is a lateral singularity at x_s in the integrand and/or its first order derivative, then the local quadrature outputs (q, e) *remain sensitive* to the occurrence of the nearby offending isolated singularity. Moreover, *slow convergence* under further symmetric subrange bisection occurs. However, *convergence acceleration* is possible by use of extrapolation techniques. Therefore, a flag *explicitly* pointing to the allowance of the activation of a convergence acceleration procedure is set.

The identification of the offending features depends on the order of questioning the integrand behaviour. Maximum gain is obtained provided features following from the specific quadrature knot distribution within the interpolatory quadrature sums of interest (*denser* towards the subrange ends and *sparser* towards its centre) are taken into account. This results in a number of hierarchichally ordered, non-commutative criteria, pertaining to any subrange $[\alpha, \beta] \subseteq [a, b]$.

1. If $f_\alpha = f(\alpha)$, $f_\beta = f(\beta)$, $f_\gamma = f(\gamma)$, $\gamma = (\beta + \alpha)/2$, define a *monotonic sequence*, then the maximum integrand variation exceeding the threshold ceiling which follows from the polynomial interpolation points to the need of exiting the computation/analysis process and to proceed to the *immediate symmetric bisection* of $[\alpha, \beta]$.

2. (*The endpoint slope consistency criterion.*) Given a sampling $\{f_0, f_1, f_2\}$ around the endpoint x_0 ($x_0 = \alpha$ or $x_0 = \beta$) of $[\alpha, \beta]$ over the abscissas set $\{x_0, x_1, x_2\}$, where x_1 and x_2 denote the two abscissas lying nearest to x_0 within the merged set of currently generated and inherited abscissas, the disagreement above some threshold among various estimates of the lateral first order derivative of $f(x_0)$ inside $[\alpha, \beta]$ may result in two possible decisions:

(a) under $|h| = |\beta - \alpha|/2 > 1$ or a non-monotonic sequence $\{f_0, f_1, f_2\}$, *immediate symmetric bisection* of $[\alpha, \beta]$ is recommended since it is expected that an insufficiently resolved integrand profile of the local quadrature knots will result over $[\alpha, \beta]$;

(b) the solution of a *boundary layer problem at x_0 inside* $[\alpha, \beta]$ is asked otherwise.

3. (*Nyquist local.*) The faithful representation of a non-monotonic integrand variation by the profile derived at the local abscissa set asks for a lower bound of the distance between two successive extrema not smaller than three quarters of the average inter-knot distance.

4. (*Nyquist global.*) The integrand profile derived at the local abscissa set is faithful if the number of counted oscillations inside it does not exceed the Nyquist threshold. The infringement of any of these two last criteria points to an *insufficiently resolved integrand profile* and asks for immediate symmetric subrange bisection.

5. (*Regularity at isolated inner extrema.*) The integrand $f(x)$ is *smooth* at the isolated extremal knot x_k provided

(I) The fine-scale approximation of the first order derivative $f'(x_k)$ gets closer to zero than its coarse-scale approximation.

(II) The curvature of $f(x)$ around x_k keeps *constant sign* irrespective of the manifold over which it is computed from second degree interpolatory polynomials within discrete neighbourhoods involving x_k.

The infringement of any of the conditions (I) and (II) points to an *irregular* extremum x_k.

The scale invariance of the diagnostic of an irregular extremum points to either a local jump, a turning point, or a singularity.

6. (*Integrand continuity inside monotonicity subranges.*) A quadrature knot x_k is assumed to belong to a neighbourhood (x_{k-1}, x_{k+1}) inside which the integrand $f(x)$ is continuous provided the magnitudes of the first order divided differences $d_{k,k-1}$ and $d_{k+1,k}$ agree with each other within some empirically defined threshold.

If this criterion is fulfilled, then the analysis is refined using

7. If the integrand profile is *monotonic* and the *curvature keeps constant sign* everywhere inside (α, β), then the activation of the local quadrature rules is accepted irrespective of the subrange width.

8. If the integrand profile is *monotonic* and the pattern of the sign of the curvature over a sequence of *three consecutive intervals* is either $+-+$ or $-+-$, then a *turning point with finite lateral derivatives* has to be resolved or disproved.

9. *Severe precision loss due to cancellation by subtraction.* If the integrand analysis at the *initialization step* of the automatic adaptive quadrature returns the result that the ratio of the quadrature sums of $f(x)$ and $|f(x)|$, computed by composite trapeze or generalized Simpson sums yields a result near to the machine epsilon with respect to the addition, then a *roundoff error flag is set* and the computation is *stopped*.

Within the Bayesian automatic adaptive quadrature, consistent subrange handling is secured by a *composite priority queue key*. The magnitude of the local quadrature error is the *primary priority* *queue key* which secures the storage of the subrange showing the largest local error at root. For a subrange in undefined state, the conventional value $e = oflow$, where $oflow$ is a value near to the machine overflow threshold. The depth of the terminal nodes in the binary subrange tree provides the *secondary priority queue key*. If a smaller depth is detected in the depth list, then the corresponding subrange is moved at the root with two important consequences: (1) systematic elimination of spurious well-conditioning diagnostics over large subranges; (2) consistent extrapolation procedure activation.

The subranges the local quadrature errors of which fall below a significance threshold are ruled out from the priority queue. This keeps the priority queue length to a minimal value.

References

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