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ПРИНЦИПЫ БАЙЕСОВСКОЙ АВТОМАТИЧЕСКОЙ АДАПТИВНОЙ КВАДРАТУРЫ

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Введение байесовского вывода в схему автоматической адаптивной квадратуры, разработанной в пакете QUADPACK, существенно увеличивает надежность вычисления интеграла в отсутствие априорных знаний о поведении функции в области интегрирования. Предложен анализ того прогресса, который достигнут к настоящему времени в этом направлении. Статья рекомендована к печати программным комитетом международной научной конференции "Математическое моделирование и вычислительная физика 2009" (MMCP2009, http://mmcp2009.jinr.ru).

Ключевые слова: численное интегрирование, автоматическая адаптивная квадратура, анализ профиля интегрируемой функции, надежность, байесовский вывод.

1. Problem statement. The evaluation of (proper or improper) one-dimensional Riemann integrals by automatic adaptive quadrature [1–3] has been implemented and is available in the most authoritative program libraries (e.g., SLATEC, IMSL, and NAG). To alleviate severe code failures in cases of practical interest [4–6], separate codes, each being able to solve a given *specific class of integrals*, have been implemented [7, 8]. It is then user's responsibility to choose an appropriate code from a library for the problem of interest.

Such an approach remains, however, useless in the case of *parametric integrals* arising in various physical models (see, e.g., [9–13]). Since the variation of the model parameters results in the occurrence of integrals falling in *different* classes, *a priori* decisions concerning the assignment of the right code cannot be taken. We are thus left with the trial and error approach, with an unacceptably high rate of failure and frustration.

If the reliability of the local quadrature rule output pairs (q, e) is explicitly questioned via the use of *post validation* consistency criteria [14, 15], then the overwhelming fraction of the *spurious* (q, e) pairs is ruled out, with the consequence that the class conscious decisions [2] of the automatic adaptive quadrature algorithms get significantly improved.

In the present paper, we discuss a set of necessary consistency criteria allowing the identification of the spurious (q, e) outputs *prior to the activation of the local quadrature rules*. This is an instance of *Bayesian inference* [16] which, by elimination of the guaranteed spurious outputs (q, e), increases the chance of obtaining meaningful (q, e) pairs under *complete lack of a priori knowledge on the integrand function*.

2. Definitions and notations.

2.1. The integral. We consider the (proper or improper) one-dimensional Riemann integral

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

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

If the integrand is *factorized* as a product $g(x)f(x)$, where the *weight function* $g(x)$ absorbs an analytically integrable difficult part of the integrand (e.g., an endpoint singular or oscillatory function), then the following considerations are equally valid for this integrand function $f(x)$.

2.2. Local quadrature rules. Given $[\alpha, \beta] \subseteq [a, b]$, a *local quadrature rule* produces an approximate solution of $I[\alpha, \beta]f$ as a couple $\{q, e\}$, where $q \equiv Q[\alpha, \beta]f$ denotes a *quadrature sum* approximation of $I[\alpha, \beta]f$, while $e > 0$ denotes a probabilistic bound of the error *(estimate of the error)* associated to q. If $e > |e_q|$, where $e_q = I[\alpha, \beta]f - q$ is the actual error associated to q, then the couple $\{q, e\}$ is *reliable*, otherwise it is unreliable. In the first case, the decisions of a class conscious automatic adaptive algorithm are *meaningful*, while in the second a *wrong* decision branch may be chosen and the numerical solution fails.

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We assume that q is a $(2n+1)$-knot *interpolatory quadrature sum* $q \equiv q_{2n} \equiv Q_{2n}[\alpha,\beta]f = \sum_{i=0}^{2n} w_i f(x_i)$ at the $2n+1$ abscissas (called the *quadrature knots*) inside $[\alpha,\beta]$:

$$\alpha \leqslant x_0 < x_1 < \ldots < x_{2n} \leqslant \beta\,. \tag{2}$$

An automatic adaptive quadrature algorithm may operate with one or more local quadrature rules. In what follows, we assume that these may be either Gauss–Kronrod (`GK`) or Clenshaw–Curtis (`CC`) quadrature rules [1–3]. Both of them result in *symmetric* quadrature sums, with the interpolation abscissas (2) given by $x_i = c + hy_i$; $c = \frac{1}{2}(\beta+\alpha)$; $h = \frac{1}{2}(\beta-\alpha)$; $i = 0, 1, \ldots, 2n$, where

$$0 = y_n < y_{n+1} < y_{n+2} < \ldots < y_{2n} \leqslant 1, \quad y_{n-i} = -y_{n+i}, \quad i = 1, \ldots, n, \tag{3}$$

denote the reduced quadrature knots y_i defined over $[-1,1]$.

2.3. Standard automatic adaptive quadrature. The automatic adaptive quadrature was systematically developed in `QUADPACK` [1], the *de facto* standard of one-dimensional globally adaptive numerical integration. A globally adaptive quadrature algorithm involves the following two fundamental steps (`QUADPACK` [1], p. 60).

(i) *Initialization:* the number of integration subranges is set to $N = 1$ and the local quadrature rule (q, e) is used to solve the given integral over the whole integration domain to yield the initial global pair $(Q_1 = q, E_1 = e > 0)$. Using Q_1 and the input accuracy specifications, an initial estimate τ_1 of the acceptable tolerance associated to the initial solution is computed.

(ii) *Error decrease by subrange subdivision:* if $E_N > \tau_N$ (i.e., the global error estimate $E_N > 0$ associated to the composite quadrature sum approximation Q_N exceeds the tolerance level τ_N), then the local quadrature errors are decreased by subrange bisection (hence, N is increased to $N+1$) and the global quantities $\{Q_N, E_N, \tau_N\}$ are updated until the error tolerance level is achieved $(E_N < \tau_N)$.

2.4. The integrand profile. The set of all currently computed values of the integrand over the current subrange $[\alpha,\beta] \subseteq [a,b]$ defines the *integrand profile* over $[\alpha,\beta]$.

Within the Bayesian automatic adaptive quadrature, the integrand profile comes from two kinds of abscissas: *inherited* from the *ancestor subranges* and the *local quadrature knots* (3) inside (α,β).

While not currently needed for the computation of the local (q,e) pair, the inherited abscissas and integrand values provide valuable enhancement of the quality of the integrand behavior analysis over $[\alpha,\beta]$.

The role of the local quadrature knots (2) or (3) is twofold. First, they serve to the derivation of hints on the integrand conditioning over $[\alpha,\beta]$. Second, under fulfillment of all the well-conditioning criteria by the integrand function, they serve to the derivation of the outputs (q,e) for the local quadrature rules.

The union of the inherited and currently computed abscissas over $[\alpha,\beta]$ defines the *fine discretization set* of abscissas over $[\alpha,\beta]$. This may be defined either in terms of $\{x_l < x_{l+1} < \ldots < x_r\}$, the absolute abscissa values, or in terms of $\{y_l < y_{l+1} < \ldots < y_r\}$, the reduced abscissa values. Both sets of abscissas are *uniquely defined* for any arbitrary subrange $[\alpha,\beta] \subseteq [a,b]$.

In what follows, the distance between two reduced abscissas will be of interest:

$$\eta_{jk} = y_k - y_j, \quad j, k \in \{l, l+1, \ldots, r\}. \tag{4}$$

2.5. Discrete neighborhoods over the integrand profile sampling. The analysis of the integrand behavior around a certain quadrature knot $x_k \in [\alpha,\beta]$ asks for the use of neighborhoods which are defined in terms of the already available integrand profile sampling. This analysis is *local* and involves several kinds of neighborhoods.

The *left fine discretization neighborhood* of x_k is given by

$$\mathcal{F}_l(x_k) = \{x_{k-2}, x_{k-1}, x_k, x_{k+1}\} \cap \{x_l, \ldots, x_r\}. \tag{5}$$

The *left coarse discretization neighborhood* of x_k is given by

$$\mathcal{C}_l(x_k) = \{x_{k-2}, x_k\} \cap \{x_l, \ldots, x_r\}. \tag{6}$$

Similar definitions hold for the right discretization neighborhoods $\mathcal{F}_r(x_k)$ and $\mathcal{C}_r(x_k)$, respectively.

The *left lateral neighborhood* of x_k is given by $\mathcal{L}_l(x_k) = \{x_{k-3}, x_{k-2}, x_{k-1}, x_k\} \cap \{x_l, \ldots, x_r\}$. The left lateral neighborhood is *complete* provided it contains exactly four points. Similar definition holds for the right lateral neighborhood $\mathcal{L}_r(x_k)$.

The inner extremal point x_k of the integrand profile is *isolated to the left* provided $\mathcal{L}_l(x_k)$ is complete and the sequence $\{f_{k-3}, f_{k-2}, f_{k-1}, f_k\}$ is *monotonic*.

An inner extremal point x_k is *isolated* provided it is isolated both to the left and to the right.

A monotonic subset of sequential integrand profile values $\{f_l, f_{l+1}, \ldots, f_{l+q}\}$ defines a *monotonicity subrange* inside $[\alpha, \beta]$ provided its length $q + 1 \geqslant 6$.

3. Integrand features subject to Bayesian inferences. There are integrand features which result in conspicuously unreliable local quadrature rule (q, e) outputs if properly questioned and identified:

— severe precision loss due to cancellation by subtraction;

— 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;

— occurrence of a finite jump with finite lateral derivatives, immersed into a monotonicity subrange of the integrand;

— same as previous, but turning point;

— integrand oscillations at a rate of variation beyond the current quadrature knot set resolving power;

— isolated irregular integrand extremum.

The specific decisions following from the identification of one or another of the above-mentioned cases depends on the diagnostic. One of the following three continuations is possible:

(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 $[\alpha, \beta] = \big[(\alpha, x_s) \cup (x_s, \beta)\big]$. 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* [17, 18] at x_s^+ or x_s^-, respectively, in order to determine the *nature* of the integrand behavior 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 neighborhood (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 the use of extrapolation techniques. Therefore, a flag *explicitly* pointing to the allowance of the activation of a convergence acceleration procedure is set.

This discussion points to the need of *three pointers* for the integrand behavior characterization over a subrange, corresponding to the left end, the right end, and the subrange interior respectively.

The pointer ipinn characterizing the *interior* of a subrange carries the output analysis information given in Table 1.

The pointer ipend characterizing *a subrange end* carries the information given in Table 2.

4. Order of integrand computation at quadrature knots over subranges. Within the standard automatic adaptive quadrature, all the integrand values asked by the local quadrature rule pair (q, e) are computed, irrespective of the meaningfulness of the (q, e) output or not.

Within the Bayesian automatic adaptive quadrature, the computation of the integrand values *and* the analysis of the integrand behavior, *prior* to the activation of the local quadrature rule, are done in separate distinct procedures. A noticeable decrease of the number of integrand evaluations may be obtained provided the analysis is done as soon as possible after the computation of a new integrand value. The computation/analysis

Table 1

ipinn	
0	All consistency criteria passed. Local quadrature rule activation allowed.
-2	Insufficiently resolved integrand profile. Do immediate symmetric bisection.
-1	Localized integrand difficulty. Solve auxiliary and/or boundary layer problems.
2	Heavy cancellation by subtraction. Stop all computations and issue error flag.

Table 2

ipend	
0	Free, presumably regular, subrange end.
1	Locked singularity in function and/or first order derivative. Allow extrapolation.
2	Locked zero measure subrange end. Extrapolation denied.
3	Essential singularity. Stop all computations and issue error flag.

process may be optimized as a two-step interlacing involving the computation of an appropriate subset of integrand values, followed by the check of corresponding consistency criteria.

The minimal subset of integral values requested by the analysis comprises the subrange ends and the inner local quadrature knots inside $(\alpha, \beta) \subseteq (a, b)$. In order to make the following discussion independent of the open (GK) or closed (CC) character of the local quadrature sum of interest, we consider the union of the quadrature knots (3) with the reduced endpoint abscissas: $\{y_{\gamma_l} < y_{\gamma_l+1} < y_{2n+\gamma_r}\} = \{y_0 < y_1 < \ldots < y_{2n}\} \cup \{-1, 1\}$. The integrand values $f_\alpha = f(\alpha)$ and $f_\beta = f(\beta)$ at the endpoints $y_{\gamma_l} = -1$ and $y_{2n+\gamma_r} = +1$ are either *inherited* from the parent subrange or computed during the *root initialization* of the *binary subrange tree*.

A consequence of the use of local quadrature sums of interpolatory type is the characteristic symmetric distribution of the quadrature knots inside every subrange $(\alpha, \beta) \subseteq (a, b)$: *sparser* towards the subrange center (such that the norm of distribution (4) is given by $\max\{|\eta_{jk}|\} = y_{n+1} = -y_{n-1}$) and *denser* towards the subrange ends (with the outermost two quadrature knots lying significantly nearer to each other and to the corresponding subrange end as compared to the remaining ones).

The average inter-knot distance

$$\bar{\nu} = (2n + \gamma_r - \gamma_l)^{-1} \tag{7}$$

provides a convenient threshold for the separation from each other of the sparse and dense knot regions respectively inside the left and right subrange halves.

The center $y_n = 0$ itself (or, in absolute units, $\gamma = (\beta + \alpha)/2$) plays a special role within the symmetric bisection since the pairs (f_α, f_γ) and (f_γ, f_β) provide endpoint inheritance for the descendent subranges.

This discussion points to a computation/analysis two stage process which is to be done for seven distinct groups of inner quadrature knots: the center of $[\alpha, \beta]$; the left and right pairs of quadrature knots lying nearest to the endpoints α and β respectively inside $[\alpha, \beta]$; the left-half and right-half subsets covering the remaining dense quadrature knot distributions; ibid., for sparse quadrature knot distributions.

Under the *inheritance* of previously computed integrand values over the ancestor ranges, the analysis process is completed by the operation of *merging* the inherited and just computed sequences with the purpose of enhancing the reliability of the Bayesian inferences.

5. Severe precision loss due to cancellation by subtraction. Following the idea first developed in QUADPACK ([1], p. 71), we formulate the following criterion which ends quickly the computation of a vanishing integral value under non-vanishing integrand.

Criterion C1. If the integrand analysis at the *initialization step* of the automatic adaptive quadrature returns the result $\sum_{k=\gamma_l}^{2n+\gamma_r} f(x_k) < 100\,\varepsilon_0 \sum_{k=\gamma_l}^{2n+\gamma_r} \big|f(x_k)\big|$, where ε_0 is the epsilon with respect to addition, then a *roundoff error flag is set* and the computation is *stopped*.

6. Upper bound to the global range of variation of a monotonic integrand. The key to the derivation of such a bound is provided by

Fact 1. Let $X_M = \max\{|\alpha|, |\beta|\}$ denote the endpoint maximum absolute value of the current quadrature

subrange $[\alpha, \beta] \subseteq [a, b]$.

The *floating point degree of precision*, K of an interpolatory quadrature sum showing an *algebraic degree of precision* equal to d is an effective value defined as follows:

$$K = \begin{cases} d & \text{iff} \quad X_M \in [x_m, x_M], \quad x_m = \varepsilon_0^{1/d}, \quad x_M = x_m^{-1}, \\ \left[\ln \varepsilon_0 / \ln X_M\right] & \text{iff} \quad X_M < x_m, \\ \left[-\ln \varepsilon_0 / \ln X_M\right] & \text{iff} \quad X_M > x_M, \end{cases}$$

where $[a]$ denotes the integer part of $a > 0$.

Proof. The result follows from the consideration of the fundamental polynomial $p_d(x) = \sum_{k=0}^{d} x^K$ and derivation of those conditions under which *all* the monomials of the fundamental power series $\{1, x, \ldots, x^K\}$ bring significant bits to the computed values of $p_d(x)$ at various arguments x.

From $p_d(x)$ it follows that 2^K is a worst case upper bound for the range of variation of the integrand values over the triplet $\{f_\alpha, f_\gamma, f_\beta\}$. We may therefore formulate

Criterion C2. Let $[\alpha, \beta] \subseteq [a, b]$, $f_\alpha = f(\alpha)$, $f_\beta = f(\beta)$, $f_\gamma = f(\gamma)$, $\gamma = (\beta + \alpha)/2$; $\Delta_{\alpha\gamma} = |f_\gamma - f_\alpha|$; $\Delta_{\gamma\beta} = |f_\beta - f_\gamma|$. If $\{f_\alpha, f_\gamma, f_\beta\}$ define a *monotonic sequence*, then the infringement of the condition

$$2^K \min\{\Delta_{\alpha\gamma}, \Delta_{\gamma\beta}\} > \max\{\Delta_{\alpha\gamma}, \Delta_{\gamma\beta}\}$$

points to the need of exiting the computation/analysis process and to proceed to the *immediate symmetric bisection* of $[\alpha, \beta]$.

7. Inferences from integrand slope approximation at a subrange endpoint.

Criterion C3 (*the endpoint slope consistency criterion*). Given:

(i) $[\alpha, \beta] \subseteq [a, b]$ and 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,

(ii) the three estimates $\widetilde{f}_0'^{(k)}$ $(k = 1, 2, 3)$ of $f_0' = f'(x_0)$ following from the samplings $S_1 = \{f_0, f_1\}$ and $S_2 = \{f_0, f_2\}$ as a first order divided difference $\widetilde{f}_0'^{(k)} = d_{k0} = \dfrac{f_k - f_0}{x_k - x_0} = \dfrac{f_k - f_0}{h\eta_{k0}}$, $k = 1, 2$, or from the sampling $S_3 = \{f_0, f_1, f_2\}$ as $\widetilde{f}_0'^{(3)} = d_{10} + (d_{10} - d_{20})\rho_{10,20}$, $\rho_{10,20} = \dfrac{\eta_{10}}{\eta_{20}}$, then the set $\left\{\widetilde{f}_0'^{(1)}, \widetilde{f}_0'^{(2)}, \widetilde{f}_0'^{(3)}\right\}$ is taken for being consistent provided

$$\left|\widetilde{f}_0'^{(1)} - \widetilde{f}_0'^{(3)}\right| \leqslant \left|\widetilde{f}_0'^{(2)} - \widetilde{f}_0'^{(3)}\right| \leqslant \tau \max\left\{\left|f_0'^{(1)}\right|, \left|f_0'^{(2)}\right|, \left|f_0'^{(3)}\right|, 1\right\}, \tag{8}$$

where τ is an empirical value set to $\tau = 1/3$.

If the consistency criterion (8) is infringed, then:

(a) under $|h| = \dfrac{|\beta - \alpha|}{2} > 1$ or a nonmonotonic sequence S_3, *immediate symmetric bisection* of $[\alpha, \beta]$ is recommended, since it is expected that an insufficiently resolved integrand profile by the set (3) 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.

8. Check of Nyquist threshold for oscillatory integrands. The reconstruction of periodic signals ([17], Chap. 12) shows that the structural details recovered by analysis cannot be finer than the norm of the discretization sampling. The Nyquist theorem established in this context has two straightforward implications in the Bayesian automatic adaptive quadrature with respect to the faithful representation of the integrand function structure by the integrand profile at the set of the local quadrature knots (3).

Criterion C4 (*Nyquist local*). The faithful representation of a non-monotonic integrand variation by the profile derived at the local abscissa set (3) asks for a lower bound of the distance between two successive extrema not smaller than $3/4\bar{\nu}$, with $\bar{\nu}$ given by (7) and $3/4$ being an empirical factor.

Criterion C5 (*Nyquist global*). The integrand profile derived at the local abscissa set (3) is faithful if the number of counted oscillations inside it does not exceed the Nyquist threshold $2/y_{n+1}$.

The infringement of any of these two criteria points to an *insufficiently resolved integrand profile* and this asks for immediate symmetric subrange bisection.

9. Integrand behavior at isolated inner extrema. If x_0 is an extremal point of a smooth function $f(x)$, then $f'(x_0) = 0$ and there is a finite neighborhood $V(x_0)$ of x_0 inside which $f''(x_0) \neq 0$. These fundamental properties result into the following Bayesian hint:

Criterion C6. The integrand $f(x)$ is *smooth* at the isolated extremal knot x_k provided

(I) $\left|f'_{\mathcal{F}}(x_k)\right| < \left|f'_{\mathcal{C}}(x_k)\right|$, where $\{\mathcal{F}, \mathcal{C}\}$ is a symbolic notation for the pairs $\left\{\mathcal{F}_l(x_k), \mathcal{C}_l(x_k)\right\}$ and respectively $\left\{\mathcal{F}_r(x_k), \mathcal{C}_r(x_k)\right\}$, Eqs. (5) and (6);

(II) the curvature of $f(x)$ at $\left\{x_{k-1}, x_k, x_{k+1}\right\}$ keeps *constant sign* irrespective of the manifold $\mathcal{L}_l(x_k)$, $\mathcal{F}_l(x_k)$, $\mathcal{F}_r(x_k)$, or $\mathcal{L}_r(x_k)$ over which it is computed from third degree interpolatory polynomials.

The infringement of any of conditions (I) and (II) points to an *irregular* extremum x_k. *Scale invariance* of the diagnostic of an irregular extremum is checked under symmetric bisection until it is detected at a half-width $|h| < 1$, therefrom the analysis follows the general pattern described at point (iii) of Section 3.

10. Checking integrand regularity over monotonicity subranges. The analysis done in this case is based [15] on the comparison of the first order divided differences $d_{k+1,k} = \dfrac{f_{k+1} - f_k}{h\eta_{k+1,k}}$ and is formalized in the following Bayesian hint:

Criterion C7. A quadrature knot x_k is assumed to belong to a neighborhood (x_{k-1}, x_{k+1}) inside which the integrand $f(x)$ is continuous provided the first order divided differences satisfy

$$\min\left\{|d_{k,k-1}|, |d_{k+1,k}|\right\} \geqslant \tau \max\left\{|d_{k,k-1}|, |d_{k+1,k}|\right\}, \tag{9}$$

where τ is an empirically defined threshold.

Under infringement of (9), the analysis follows the general pattern (iii), Section 3.

If Criterion C7 is fulfilled, then the analysis is refined using

Criterion C8. 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.

Criterion C9. 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.

11. Mesoscopic analysis of the boundary layer [17, 18]. Assume that $f(x)$ is a continuous twice differentiable function over $[a, b]$ and let $x_r \in [a, b]$ denote a reference argument value. Then there exists a non-vanishing neighborhood $V(x_r) \subseteq [a, b]$ of x_r inside which a *linear* Taylor series expansion holds true within a predefined threshold $0 < \varepsilon \ll 1$.

Numerical check of the continuity of $f(x)$ is done from a *sampling of its computed values*,

$$\Big\{f_i = fl\big(f(x_i)\big) \,\Big|\, i = 0, 1, \ldots, m\Big\},$$

over a set of machine number arguments $S_m(x_r) = \left\{x_i \in V(x_r) \,\middle|\, i = 0, 1, \ldots, m\right\}$, $m \geqslant 3$, chosen such that $fl(x_r) \in S_m(x_r)$, where $fl(\zeta)$ denotes the floating point representation of $\zeta \in \mathbb{R}$. Let $\left\{f(x_i) \,|\, i = 0, 1, \ldots, m\right\}$ denote the set of *actual* values of $f(x_i)$ over $S_m(x_r)$. In general, due to the round-off, $f(x_i) - fl\big(f(x_i)\big) \neq 0$, hence the best information on the smoothness properties of $f(x)$ at x_r following from the set $\left\{x_i, f_i\right\}$ is obtained from the scrutiny of the properties of a second degree polynomial least squares fit to the floating point data.

It is convenient to perform the *scale transformation* $x_i = x_0 + \xi_i h_r$, $i = 0, 1, \ldots, m$, $\xi_i \in \mathbb{Z}$, where h_r denotes the distance from x_r to its nearest machine number inside $[a, b]$. This leads to the second degree fitting polynomial $y_2(x_i) = \alpha_0 + \alpha_1 h_r p_1(\xi_i) + \alpha_2 h_r^2 p_2(\xi_i)$, spanned by the orthogonal basis polynomials $p_k(\xi_i)$, $k = 0, 1, 2$, of norms N_k, respectively. Under negligible α_2, the first order derivative of $f(x)$ at x_r is given by $f'(x_r) \approx y'_2(x_r) = \alpha_1 = N_1^{-1} \sum\limits_{i=0}^{m} p_1(\xi_i) f_i$.

The smallest sampling $S_m(x_r)$ suitable for a least squares analysis providing insight on the smoothness properties of $f(x)$ at $x_r = a$ and $x_r = b$ respectively consists of four distinct abscissas (i.e., $m = 3$). We choose them such that the set $\{x_0, x_1, x_2\}$ defines a *uniform mesoscopic mesh* $\xi_0 = 0$, $\xi_1 = p$, $\xi_2 = 2p$, $\xi_3 = q$, $q \neq \{0, p, 2p\}$.

Then the validity of a linear Taylor expansion around the reference abscissa x_r is found to hold true within prescribed accuracy ε provided the minimal sampling yields *scale invariant* approximations of the first order derivative $f'(x)$. Details and implementation are reported in [17, 18].

12. The priority queue associated to the binary subrange tree. Within the standard automatic adaptive quadrature, the magnitude of the local quadrature error e provides the simple key pointing to the subrange to be bisected next.

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.

13. Conclusions. A review of the principles of the Bayesian automatic adaptive quadrature has been given. Special emphasis was put on the description of the integrand properties which result in conspicuously unreliable local quadrature rule (q, e) outputs *prior* to their effective computation. Consistency criteria enabling Bayesian hints are formulated. Detailed considerations of such criteria in separate publications pointed to the substantial increase of the reliability of the automatic globally adaptive quadrature under their use.

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References

1. *Piessens R., deDoncker-Kapenga E., Überhuber C.W., Kahaner D.K.* `QUADPACK`, a subroutine package for automatic integration. Berlin: Springer Verlag, 1983.
2. *Davis P.J., Rabinowitz P.* Methods of Numerical Integration, Second edition. Orlando (Fla), USA: Academic Press, 1984.
3. *Krommer A.R., Ueberhuber C.W.* Computational Integration. Philadelphia: SIAM, 1998.
4. *Lyness J.N.* When not to use an automatic quadrature routine // SIAM Rev. 1983. **25**. 63–87.
5. *Adam Gh., Nobile A.* Product integration rules at Clenshaw–Curtis and related points: a robust implementation // IMA J. Numerical Analysis. 1991. **11**. 271–296.
6. *Adam Gh.* Case studies in the numerical solution of oscillatory integrals // Romanian J. Phys. 1993. **38**. 527–538.
7. NAG Ltd., NAG Fortran Library Manual — Mark 17, Oxford, UK, 1996.
8. Visual Numerics Inc., IMSL MATH/LIBRARY: User's Manual — Version 3.0, Houston, TX, 1994.
9. *Plakida N.M., Anton L., Adam S., Adam Gh.* Exchange and spin-fluctuation mechanisms of superconductivity in cuprates // Zh. Exp. Teor. Fiz. 2003. **124**. 367–378; English transl.: J. Exp. Theor. Phys. 2003. **97**. 331–342.
10. *Marchetti P.A., Zhao-Bin Su, Lu Yu* $\mathrm{U}(1) \times \mathrm{SU}(2)$ Chern–Simons gauge theory of underdoped cuprate superconductors // Phys. Rev. B 1998. **58**. 5808–5824.
11. *Marchetti P.A., Jian-Hui Dai, Zhao-Bin Su, Lu Yu.* Gauge field theory of transport and magnetic relaxation in underdoped cuprates // J. Phys.: Cond. Matter 2000. **12**. L329–L336.
12. *Chu C.W.* High Temperature Superconducting Materials: Present Status, Future Challenges, and One Recent Example — the Superconducting Ferromagnet // Physica C 2000. 341–348. 25–30.
13. *Săndulescu A., Mişicu ,S., Cârstoiu F., Florescu A., Greiner W.* Role of the higher static deformation of fragments in the cold binary fission of ^{252}Cf // Phys. Rev. C 1998. **57**. 2321–2328.
14. *Adam Gh., Adam S.* Increasing reliability of Gauss–Kronrod quadrature by Eratosthenes' sieve method // Computer Phys. Commun. 2001. **135**. 261–277.
15. *Adam Gh., Adam S.* Reliability Conditions in Quadrature Algorithms // Computer Phys. Commun. 2003. **154**. 49–64.
16. *Justice J.H.* Maximum Entropy and Bayesian Methods in Applied Statistics. Cambridge: Cambridge University Press, 1986. *E.T. Jaynes.* Bayesian methods: An introductory tutorial.
17. *Adam Gh., Adam S., Tifrea A., Neacsu A.* Resolving thin boundary layers in numerical quadrature // Romanian Reports in Physics. 2006. **58**, N 2. 107–122.
18. *Adam Gh., Adam S.* The boundary layer problem in Bayesian adaptive quadrature // Physics of Particles and Nuclei Letters. 2008. **5**, N 3. 269–273.
19. *Press W.H., Teukolsky S.A., Vetterling W.T., Flannery B.P.* Numerical Recipes in Fortran 77 — The Art of Scientific Computing. Second Edition. Cambridge: Cambridge University Press, UK, 2001.

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