Dedicated to Professor Mihai Gavrilă's 80th Anniversary

FLOATING POINT DEGREE OF PRECISION OF AN INTERPOLATORY QUADRATURE SUM

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Received December 18, 2009

The Bayesian approach to the automatic adaptive quadrature enhances the reliability of the local quadrature rules using a number of consistency criteria which enable the detection of spurious integrand profiles prior to the activation of the local quadrature rules. The present paper discusses a number of criteria which make heavy use of the floating point degree of precision of a local quadrature sum and of averages based on the composite trapeze sum (an upper bound to the allowable range of variation of the integrand, early termination in case of severe cancellation by subtraction, automatic cutoff of an infinite integration domain).

1. INTRODUCTION

The present paper is devoted to the derivation or refinement of a number of *a priori* conditioning diagnostics of the integrand in the Bayesian automatic adaptive quadrature [1].

The motivation of the need of Bayesian automatic adaptive quadrature algorithms comes from the fact the standard automatic adaptive quadrature ones (see, e.g., the discussion in the monographs [2, 3, 4]) show a high degree of failure when used for extensive computations of observables in physical models describing systems with intricate phase diagrams. Consider for instance the high critical temperature superconducting phase transitions in cuprates which critically depend on the degree of doping with holes or electrons of the reference stoichiometric structures (for a recent extensive review of this puzzle of the last two and a half decades of the solid state physics see [5]). Their numerical investigation within the two-band Hubbard model (see [6, 7, 8] and references therein) is hindered by the

impossibility to know in advance the right integrand behaviour and to secure in this way safe algorithm choices from the menus offered by the existing program libraries SLATEC, IMSL, or NAG.

To make clear the need of the *a priori* conditioning diagnostics, the discussion starts with an outline of the Bayesian approach to the automatic adaptive quadrature in section 2. The following discussion uses heavily the concept of *floating point degree of precision* of a quadrature sum, which is articulated in section 3. Each of the next three sections deals with a specific conditioning diagnostic. In section 4 it is shown that the mere knowledge of the integrand values at the ends of a finite integration subrange and at its centre enables a first decision on the usefulness of proceeding to the further derivation of the information required by the local quadrature sum to compute a reliable approximation of the integral or on the need to stop immediately this process and to proceed to the definition of descendents by symmetric bisection of the subrange. Section 5 solves the problem of early detection of a vanishing value of the integral over a finite range. This quest provides a reference threshold which allows the derivation of a reliable automatic cutoff of an infinite integration domain, in section 6. The paper ends with conclusion in section 7.

2. OUTLINE OF THE BAYESIAN AUTOMATIC ADAPTIVE QUADRATURE

The integral to be solved numerically is the (proper or improper) one-dimensional Riemann integral,

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

Here $\left[a,b\right] \subseteq \mathbb{R}$, denotes the integration domain, while the integrand function $f:\left[a,b\right] \to \mathbb{R}$ 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., endpoint singular or oscillatory function), then the following considerations are equally valid for this integrand function *f(x)*.

The integral (1) is solved within a prescribed accuracy $\tau > 0$ provided an approximate value Q of I is computed together with an estimate $E > 0$ of the error associated to Q such that

$$\left|I - Q\right| < E < \tau \tag{2}$$

If the condition $E < \tau$ is not fulfilled, the value of Q is refined, hence the error estimate E is lowered, until (2) is satisfied.

One way to reach this goal uses the automatic adaptive quadrature approach. Within it, *a subrange subdivision strategy* is used. It produces the division of a suitable chosen subrange $[\alpha,\beta]\subseteq[a,b]$ into two equal subranges. Such a procedure generates a *binary subrange tree* the root of which is the original integration domain [*a,b*]. Over each descendent [*α,β*] within the binary subrange tree, *local pairs (q,e)* are built using local specific *quadrature sums q* and *error estimates e* > 0. The *local quadrature rule* results are then summed to yield the global quantities (*Q,E*) entering the global termination criterion (2).

In (2), the specification of τ makes use of two parameters [2]: the absolute accuracy ε_a and the relative accuracy ε_r, such that

$$\tau = \max\left\{\varepsilon_a, \varepsilon_r |I|\right\} \simeq \max\left\{\varepsilon_a, \varepsilon_r |Q|\right\}. \tag{3}$$

The equations (2) and (3) unveil the occurrence of delicate reliability problems of the output characterization.

First, the practical specification of the accuracy τ in (3) points to the fact that the reliability of the accuracy characterization depends on the quality of *Q*, the derived approximation to the input integral *I*.

Second, the error estimate *E*, the derivation of which is done based on probabilistic arguments, may be reliable or not, hence there is not guarantee that the decision to end the computations is unconditionally safe.

In fact, there is a long term evidence [9]–[11] that the standard automatic adaptive quadrature approach may yield spurious outputs: wrong results which carry the diagnostic of providing safe solutions may be generated. The recipe proposed to cure this drawback of the standard approach was to implement into computer codes several automatic adaptive algorithms each of which is able to solve a *specific class* of integrals (1). It was then assumed that the user will choose the right code from the proposed menu. As mentioned in the introduction, such an approach fails in the numerical investigation of phase transition models involving some continuously varying parameter which may result in drastic change of the integrand behaviour, such that it is impossible to decide in advance what code to use.

In order to overcome this dead end of the standard automatic adaptive quadrature, we have proposed at the ICCAM 2004 Conference [12] a substantiated approach based on principles of the Bayesian inference.

The Bayesian approach preserves the two basic principles of the automatic adaptive quadrature (a subrange subdivision strategy combined with the use of local quadrature rules). However, their practical implementation is substantially modified [1].

The priority queue associated to the binary subrange tree automatically activates the subdivision of the significant subrange of the largest width, such that the uncertainties related to the coarser information are automatically damped out and a singular subrange is brought at the root of the priority queue just at the right moment.

The most difficult part of the Bayesian approach concerns the activation of the local quadrature rules. In contradistinction to the standard approach, there is not allowance for their activation unless a number of hierarchically ordered well-conditioning criteria are satisfied. In this way, the probability of having at hand significant reliable local pairs (q,e) is brought near a hundred percent certainty, or the occurrence of a difficult point hindering the derivation of the correct output is adequately characterized.

The quality of the analysis is enhanced by the fact that the available *integrand profile* over the descendent subranges in the binary subrange tree consists of both *newly computed integrand values* at the current quadrature knots and *inherited integrand* values (together with the corresponding abscissas) from their ancestor subranges.

While the general characterization of the Bayesian approach is clear, there are still details of its implementation which need scrutiny. Henceforth we shall discuss topics following from the *floating point degree of precision* of a quadrature sum.

3. FLOATING POINT DEGREE OF PRECISION

A $(2n+1)$-knot interpolatory quadrature sum $q_d[\alpha, \beta]f$ approximates the solution of $I[\alpha, \beta]f$ by

$$q_d\left[\alpha,\beta\right]f = I\left[\alpha,\beta\right]p_d \tag{4}$$

where $p_d(x)$ is an algebraic polynomial the values of which equate those of the integrand function $f(x)$ at the quadrature knots x_i,

$$p_d\left(x_i\right) = f\left(x_i\right), \qquad i = 0, 1, ..., 2n\,. \tag{5}$$

The Gauss-Kronrod (GK) and Chebyshev-Curtis (CC) quadrature sums, which are spanned by specific sets of orthogonal polynomials, are the most frequently used for the derivation of local quadrature rules [2] (see also [10]). Having this in mind, we consider henceforth *symmetric* $(2n + 1)$-knot local quadrature sums over $\left[\alpha,\beta\right]\subseteq\left[a,b\right]$, with the interpolation abscissas given, in symmetric notation, by

$$x_i = c + hy_i;\ c = \left(\beta+\alpha\right)/2;\ h = \left(\beta-\alpha\right)/2;\ i = -n, -n+1, ..., n. \tag{6}$$

where

$$0 = y_0 < y_1 < ...y_n \le 1, \quad y_{-i} = -y_i, \quad i = 1, ..., n, \tag{7}$$

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

The quadrature sum (4) satisfies

$$q_d\left[\alpha,\beta\right]x^k = I\left[\alpha,\beta\right]x^k, \quad \forall k \in \{0,1,...,d\}, \quad \forall\left[\alpha,\beta\right]\subseteq\left[a,b\right] \tag{8}$$

Definition 1. *The maximum degree d at which (8) is fulfilled denotes the* algebraic degree of precision *of the quadrature sum $q_d[\alpha,\beta]f$.*

Remark 1. *Under calculations over the field $\mathbb{R}$ of the real numbers, the algebraic degree of precision d* is independent on the integration limits *α and β.*

This follows from the fact that the calculations of x^k over $\mathbb{R}$ are performed and taken into account *exactly*, irrespective of the argument $x \in \left[\alpha,\beta\right]$.

Definition 2. *Assume that the floating point computation of the quadrature sum $q_d[\alpha,\beta]f$ over the finite subrange $[\alpha,\beta] \subseteq [a,b]$ is done over a floating point machine number set characterized by a t-bit binary register significand.*
Then the floating point degree of precision *of $q_d[\alpha,\beta]f$ is an integer $K \le d$ which depends on the quantity $\xi = \max\{fl|\alpha|, fl|\beta|\}$ as follows*

$$K = \begin{cases} d & \text{iff} \quad \xi \in \left[x_m, x_M\right] \\ \left[\ln \varepsilon_0 / \ln \xi\right] & \text{iff} \quad \xi < x_m \\ \left[-\ln \varepsilon_0 / \ln \xi\right] & \text{iff} \quad \xi > x_M \end{cases} \tag{9}$$

where

$$x_m = \varepsilon_0^{1/d}, \quad x_M = x_m^{-1}, \quad \varepsilon_0 = 2^{-t}. \tag{10}$$

Here fla denotes the floating point approximation of $a \in \mathbb{R}$ and [a] denotes the ceiling of fla.

The definition can be straightforwardly justified for *canonical form integrals*,

$$J\left[a,b\right]f = \int_a^b f\left(x\right)dx, \ 0 \le a < b. \tag{11}$$

Then the fundamental power sequence $\{1, x, \cdots, x^d\}$ is *strictly monotonic* for any $x \in \left[a,b\right], \ x \ne 1$.

A particular monomial of this sequence is *relevant* for the *t*-bit floating point computation of the *d*-degree polynomial

$$p_d\left(x\right) = \sum_{k=0}^{d} c_k x^k, \quad \left(c_k \ne 0, \forall k \in \{0,1,...,d\}\right), \tag{12}$$

provided

$$fl\left(1.0 + fl\left(x^k\right)\right) \ne 1.0 \quad \text{iff } fl\left(x\right) < 1.0 \tag{13}$$

and

$$fl\left(1.0 + fl\left(x^k\right)\right) \neq fl\left(x^k\right) \quad \text{iff } fl\left(x\right) > 1.0 \tag{14}$$

From these constraints it follows that *all* the $d+1$ terms in (12) are relevant provided $x_m \leq x \leq x_M$, with x_m and x_M defined in (10).

If $\xi < x_m$, then (13) is infringed for monomials x^k of degrees $K < k \leq d$, with the threshold K defined in (9). Similarly, if $\xi > x_M$ then (14) is infringed for monomials x^k of degrees $K < k \leq d$, with K defined in (9).

If zero is an inner point of the integration domain $[\alpha, \beta]$, then the floating point degree of precision can be taken for the largest values obtained for the ranges $[0,|\alpha|]$ and $[0, \beta]$. The definition is completed.

Remark 2. *At $\xi > 1$, the decrease of the floating point degree of precision with increasing ξ as shown in (9) provides a quantitative description of the empirical observation that the reliability of the integrand profile decreases over large finite integration ranges $[\alpha, \beta]$ due to two features. First, the larger the width of $[\alpha, \beta]$, the sparser is the quadrature knot distribution inside it, hence the possibility to miss important integrand features increases within the generated integrand profile. Second, since the distance between two consecutive machine numbers is proportional to their absolute values, over integration ranges $1 \ll \alpha < \beta$, the requirement to get quadrature knots described by distinct machine number inside $[\alpha, \beta]$ introduces a non-negligible lower bound to the range width, which may become large in absolute value and, as consequence, it turns to generate a poor quality integrand profile at the current set of quadrature knots.*

At $\xi < 1$, the floating point degree of precision (9) decreases with decreasing ξ value. This time, the behaviour of K is related to the radius of validity of the Taylor series expansion of a smooth enough function f(x) around x =0 within the t-bit machine register accuracy.

Remark 3. *The argument which provided the definition (9) of the floating point degree of precision K used the canonical form (11) of a Riemann integral. An arbitrary Riemann integral (1) can always be represented either as a single canonical integral (11) (if $\alpha\beta \geq 0$ or $\alpha + \beta = 0$) or as a combination of two canonical integrals (if $\alpha\beta < 0$ and $\alpha + \beta \neq 0$). The question then naturally arises on the usefulness of replacing the input integral (1) by canonical integrals.*

To settle this question, we shall make recourse to the evidence provided by the physical models. Since a system specific symmetry is almost universally explicitly present in these models, this is encompassed in the input integral (1) by the occurrence of parity properties of the integrand f(x)(often in the presence of a weight function g(x)). The integral (1) should then occur already in the canonical form (11), or the condition $\alpha + \beta = 0$ should be present both for finite or infinite integration domains. In the case of a doubly infinite integration domain, the

presence of the Coulomb interaction may ask for the definition of $I[-\infty,+\infty]f$ as a Cauchy principal part integral.

Under $\alpha + \beta = 0$, a duly formulated input integral should be provided to the automatic adaptive algorithm as a canonical integral. However, if this is not case, the implementation of the Bayesian automatic adaptive quadrature for input $I[-a,a]f$ integrals foresees inner reduction to a canonical integral. In this case, the occurrence of the cancellation by subtraction (see section 5) is detected pointwise, at each quadrature knot of the integrand of the resulting canonical integral.

4. THE LARGEST RELATIVE VARIATION OF AN INTEGRABLE FUNCTION OVER A FINITE RANGE

Let $[\alpha,\beta]$ denote a finite subrange over which a canonical integral $J[a,b]f$, Eq.(11), is to be computed.

The integrand values $f_\alpha = f(\alpha)$ and $f_\beta = f(\beta)$ at the endpoints of $[\alpha, \beta]$ are *inherited* from the parent range of $[\alpha, \beta]$. In this section we show that the computation of $f_\gamma = f(\gamma)$ at the centre $\gamma = (\beta + \alpha)/2$ of $[\alpha, \beta]$ allows the derivation of a Bayesian inference concerning the usefulness of the computation of $J[\alpha, \beta]f$ by the quadrature sum $q_d[\alpha, \beta]f$.

Assume that $\{f_\alpha, f_\gamma, f_\beta\}$ defines a strictly monotonic sequence, i.e.,

$$\Delta_{\alpha\gamma} = f_\gamma - f_\alpha,\ \Delta_{\gamma\beta} = f_\beta - f_\gamma,\ \Delta_{\alpha\gamma} \cdot \Delta_{\gamma\beta} > 0. \tag{15}$$

Denote

$$\Delta_m = \min\{|\Delta_{\alpha\gamma}|,|\Delta_{\gamma\beta}|\},\ \Delta_M = \max\{|\Delta_{\alpha\gamma}|,|\Delta_{\gamma\beta}|\}. \tag{16}$$

If $J[\alpha, \beta]f$ is well approximated by $q_d[\alpha, \beta]f$, then the ratio Δ_m/Δ_M cannot be arbitrarily small. It is necessarily bounded from below by the similar ratio $\rho_K = \delta_m/\delta_M$ following from the polynomial of the fastest variation within the class $\mathcal{P}_K$ of the polynomials of degree at most K over $[\alpha, \beta]$.

Since the polynomial of interest showing the fastest relative variation over $[\alpha, \beta]$ is x^K, we get $\delta_m = \delta_{\alpha\gamma} = \gamma^K - \alpha^K$, $\delta_M = \delta_{\gamma\beta} = \beta^K - \gamma^K$.

For an arbitrary integral (1) containing the abscissa $x = 0$ as an inner point of $[\alpha, \beta]$, the bound $\rho_K = 2^{-K}$ formulated in [1] is convenient.

Collecting together these results, we may write

$$\rho_K = \begin{cases} \left(\dfrac{\gamma}{\beta}\right)^K \left[1 - \left(\dfrac{\alpha}{\gamma}\right)^K + \left(\dfrac{\gamma}{\beta}\right)^K - \left(\dfrac{\alpha}{\beta}\right)^K\right] & \text{iff} \quad \alpha\beta \geq 0 \\ 2^{-K} & \text{otherwise} \end{cases} \tag{17}$$

We have therefore derived the following consistency criterion for a monotonic integrand (MONI).

Consistency criterion MONI. If the triplet $\{f_\alpha, f_\gamma, f_\beta\}$ of integrand values computed at the ends α, β and the centre γ of a finite integration range defines a strictly monotonic sequence, then a necessary well-conditioning criterion for the reliable approximation of $I[\alpha, \beta]f$ by the quadrature sum $q_d[\alpha, \beta]f$ of floating point degree of accuracy equal to K over $[\alpha, \beta]$ is

$$\Delta_m > \rho_K \Delta_M \tag{18}$$

where Δ_m and Δ_M are defined by the equations (15)–(16) and ρ_K by (17).

Remark 4. *If f_γ is a local extremal point (i.e., $\Delta_{\alpha\gamma}\Delta_{\gamma\beta} < 0$), then the criterion (18) is irrelevant. In this case, criteria counting the number of integrand oscillations inside $[\alpha, \beta]$ have to be invoked [1].*

Remark 5. *If the criterion (18) is infringed, then the further computation of the integrand values at inner quadrature knots is to be stopped.*

The subrange $[\alpha, \beta]$ is to be immediately subdivided into two descendents, $[\alpha,\gamma]$ (which inherits f_α and f_γ as endpoint integrand values) and $[\gamma, \beta]$ (which inherits f_γ and f_β as endpoint integrand values) respectively.

5. EARLY DETECTION OF A VANISHING INTEGRAL VALUE

If the analysis pertains to the root $[a,b]$ of the binary subrange tree and all the well-conditioning criteria have been fulfilled, then a last check before the activation of the local quadrature rule of interest concerns the quest for the possible vanishing of the value of the integral $I[a,b]f$ as a result of the heavy cancellation by subtraction of non-vanishing integrand values. This question was solved in QUADPACK [2], by computing simultaneously $q_d[a,b]f$ and $q_d[a,b]|f|$ and checking whether $q_d\left[a,b\right]f < 100\bar{\varepsilon}_0 q_d\left[a,b\right]\left|f\right|$ or not (with $\bar{\varepsilon}_0$ denoting the RAM epsilon with respect to addition).

In this section we propose an alternative criterion based on the use of simple composite quadrature sums.

The integrand profile over $[a,b]$ consists of a set of $2m+1$ integrand values $f_k = f(x_k)$ computed at the symmetrically distributed quadrature knots (6)–(7) around the centre of $[a,b]$, possibly completed with f_a and f_b in the case of an open local quadrature sum. As a consequence, we have $m = n$ for the CC-like sums and $m = n+1$ for the GK-like sums.

The simplest answer to the question of the possibly vanishing $I[a,b]f$ is provided by the use of average integrand values based on the composite trapeze sum:

$$\bar{f}_t = \frac{1}{2}\sum_{i=0}^{m}{}'' \left(f_i + f_{i-1}\right) y_{i-1,\,i+1}, \quad y_{ij} = y_j - y_i, \tag{19}$$

where $\sum''$ points to the fact that, at $i = 0$, $y_{-1,1}$ is to be replaced by $y_{01} = y_1$, while at $i = m$, $y_{m-1,m+1}$ is to be replaced by $y_{m-1,m} = 1 - y_{m-1}$.

Termination criterion ROFF. If the computation of the averages of a non-vanishing integrand $f(x)$ and of its modulus $|f(x)|$ by the composite trapeze-like sum (19) yields the result

$$\overline{f}_t < 100\overline{\varepsilon}_0 \left|\overline{f}\right|_t , \tag{20}$$

then the use of the local quadrature rule (q,e) of interest over $[a,b]$ is expected to yield the output of a vanishing integral $I[a,b]f$ due to heavy cancellation by subtraction.

Remark 6. *An alternative to the composite trapeze sum might had been provided by a composite sum following from a Simpson-like sum for non-central inner abscissa [13]. We have skipped it due to the more cumbersome form of this composite sum.*

6. ASYMPTOTIC TAILS

If (1) defines an improper Riemann integral over a (semi)infinite integration domain, then the convergence of $I[a,b]f$ asks for a sufficiently rapid decrease to zero of $f(x)$ towards the infinite end(s). Classical results are known concerning, e.g., the conditions of convergence of the Fourier transform and the Laplace transform integrals.

The physical models provide a great many number of improper Riemann integrals involving various decay behaviours of the potential at infinity: fast (screened Coulomb, Gaussian), mild (Lenard-Jones, van der Waals), slow (centrifugal), very slow (Coulombian), oscillatory damped (e.g., superexchange). Particular cases have been investigated in specific contexts in the past and very cumbersome algebraic manipulations have often been shown to be needed to get accurate solutions (see, e.g., [14] for the numerical evaluation of three-centre nuclear attraction integrals and [15] for the evaluation of multicenter two-electron Coulomb and exchange integrals over Slater functions).

However, to our best knowledge, a general approach to the consistent definition of a finite cutoff of the Riemann integrals over infinite domains was not previously undertaken within the automatic adaptive quadrature.

In the sequel we show that such an approach can be consistently implemented into an algorithm using the following basic ingredients:

(i) Splitting the original infinite integration domain $[a,b]$ into finite subranges:

$$[a,b] = \bigcup_{l=0}^{\infty} [\alpha_l, \beta_l], \quad \alpha_{l+1} = \beta_l, \quad h_l = 2h_{l-1}. \tag{21}$$

(ii) Ending the computation at the $(L+1)$-th range $[\alpha_{L+1},\beta_{L+1}]$ if the termination condition is fulfilled

$$\left|\overline{f}\right|_t^{L+1} < \tau \left|\overline{f}\right|_t^{M}, \ \tau = \max\left\{10^{-2}\varepsilon_r, 10^{2}\overline{\varepsilon}_0\right\}, \tag{22}$$

where $\left|\overline{f}\right|_t^{M}$ denotes the maximum average value (19) of $|f(x)|$ over the ranges $[\alpha_l,\beta_l]$, $l = 0, 1, \cdots, L$, defined until now.

The criterion (22) effectively solves improper Riemann integrals for fast and mild decreasing $f(x)$.

(iii) Check the occurrence of a slowly decaying asymptotic behaviour $Cx^{-\kappa}$ of the integrand over the infinite tail $[\beta_L,\infty)$. The knowledge of K_L, the floating point degree of precision of the quadrature sum $q_d[\alpha_L,\beta_L]f$ imposes the bound $1 < \kappa \le K_L$.

A least squares fit, within the accuracy τ defined in (22), of Cx^{κ} to the integrand values at the quadrature knots inside $[\alpha_{L+1},\beta_{L+1}]$ allows the confident derivation of the contribution of the tail $[\beta_L, \infty)$ to $I[a,b]f$ for a monotonic integrand.

(iv) The condition of doubling the width h_l of $[\alpha_l,\beta_l]$ with respect to the width h_{l-1} of $[\alpha_{l-1}, \beta_{l-1}]$ in (21) effectively reaches the asymptotic cut off for the fast enough decaying integrands.

However, if a slow convergence is noticed and the least squares fit to Cx^{κ} is unsatisfactory, then a *convergence acceleration* algorithm is to be invoked to reach quick end of the computations.

7. CONCLUSIONS

The Bayesian automatic adaptive quadrature performs the analysis of the properties of the gradually generated integrand profile over a finite integration range prior to the activation of the local quadrature rules. The use of conditioning criteria based on the Bayesian inference allows the identification of the presence of integrand feature which would spoil the output of the local quadrature rule. It results either in the generation of a binary subrange tree the descendents of which satisfy a basic set of well-conditioning criteria, or in the explicit identification of a feature of the integrand which prevents the derivation of a reliable numerical output.

To this aim, adequate knowledge of the basic properties of an interpolatory quadrature sum $q_d[\alpha, \beta]f$ which approximates the integral $I[\alpha, \beta]f$, Eq. (1) is needed.

The scrutiny of the algebraic degree of precision d of $q_d[\alpha, \beta]f$ points to the fact that, in floating point computation, it ceases to be independent on the location of the integration range $[\alpha, \beta]$ on the real axis. The dependence of the *floating point degree of precision*, K, of q_d on the bounds α and β of the integration range was established in Eq. (9) (Sec. 3).

Then, if the sequence $\{f_\alpha f_\gamma f_\beta\}$ of the integrand values at the range ends α, β and its centre γ is strictly monotonic, a necessary condition to get a reliable q_d output is the fulfillment of the requirement that the range of variation inside this

sequence cannot exceed the upper bound defined by the range of variation of the polynomial functions of degree at most K (the well-conditioning criterion MONI, Sec. 4).

The comparison of the average values of $f(x)$ and $|f(x)|$ over the original integration domain $[a,b]$, obtained from composite trapeze-like quadrature sums, allows the derivation of a criterion of early termination of the computations in the case of heavy cancellation by subtraction resulting in a vanishing integral $I[a,b]f$ for non-vanishing $f(x)$ (termination criterion ROFF, Sec. 5).

If the input Riemann integral is to be computed over an infinite integration domain, then consistent definition of a convenient, integrand dependent, finite cutoff is possible using trapeze-like averages and the floating point degree of precision (Sec. 6).

The derivation of further Bayesian inferences using the floating point degree of precision of a quadrature sum and trapeze-like averages is under investigation and results will be reported in the near future.

Acknowledgments. It is a pleasure to express our deep gratitude to Professor Mihai Gavrilă, whose lectures on quantum mechanics and special chapters in mathematics were among the best we ever listened and profoundly influenced our future development as scientists.

Partial financial support from the Romanian Authority for Scientific Research (Project CONDEGRID 12 EU/02.04.2009) is acknowledged.

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