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**INCREASING RELIABILITY OF GAUSS-KRONROD QUADRATURE
BY ERATOSTHENES' SIEVE METHOD**

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Abstract

The reliability of the local error estimates returned by the Gauss-Kronrod quadrature rules can be raised up to the theoretical 100% rate of success, under error estimate sharpening, provided a number of natural validating conditions are required. The self-validating scheme of the local error estimates, which is easy to implement and adds little supplementary computing effort, strengthens considerably the correctness of the decisions within the automatic adaptive quadrature.

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1 Introduction

In many instances, the observables of the theoretical models are expressed as specific integrals which, except for some limiting cases, cannot be solved analytically. The use of numerical algorithms (see, e.g., [1] for details on the available algorithms and a recent review of numerical quadrature) usually allows the derivation of accurate numerical results. Occasional bad failures of the available software may prevent extensive exploration of the predictions of intricate models. The $U(1) \times SU(2)$ gauge theory model of underdoped cuprate superconductors [2] was recently solved approximately within some simplifying assumptions [3]. However, the obtained meaningful physical solution could not be recovered from outputs generated by the available implementations of quadrature algorithms.

The present investigation was primarily motivated by the wish to solve the above mentioned model over a large range of variation of the physical parameters. The technical results reported below refer to topics of general interest which are expected to provide hints to the solution of similar difficulties met by other users of quadrature algorithms as well.

A modern quadrature algorithm usually performs automatic quadrature, the output of which consists of a pair $\{R, E\}$, where R is a computed approximation to the value I of the integral of interest, while E is an estimate of the error associated to R , thought to bound from above $|I - R|$, the modulus of the difference between the exact and computed values of the integral.

The computation of the global error estimate E is attempted as the sum of the *local error estimates* over the various subintervals generated by subrange subdivision. The quality of the implemented local error estimates influences, to a large extent, both the efficiency and the reliability of an automatic algorithm, either adaptive or non-adaptive.

A simple local error estimate, proposed by Kronrod [4], is based on the comparison of two quadrature approximations. Empirical evidence accumulated on various classes of integrals showed, however, that the genuine Gauss-Kronrod (GGK) error estimate is not very reliable. More sophisticated local error estimating algorithms have subsequently been devised [5, 6, 7]. Particularly successful automatic Gauss-Kronrod (GK) quadrature algorithms with improved local error estimates have been reported in QUADPACK [8], which has been incorporated in most major program libraries. Further studies [9] showed that a general frame for the derivation of local error estimates is offered by the sequence of orthogonal null rule approximations which can be built from the integrand values at the quadrature knots. In [9] it was also shown that the heuristic QUADPACK-GK (QDP) local error estimate can be viewed as a simplified null rule error estimate.

The present paper reports some rules of thumb which have been found to be very effective in increasing the output reliability of the automatic adaptive quadrature algorithms based on QDP local error estimates. In the next section we give the basic definitions and notations of the quantities of interest. In section 3 a summary of the main results derived in this paper

is given. In sections 4 and 5, we discuss the numerical evidence on error estimate outputs from elementary integrals of continuous monotonic functions and non-monotonic (oscillatory) functions respectively. Each kind of investigated integrand is found to add specific hints to the reliability of the derived error estimates. Some summarizing comments are given in section 6.

2 Definitions and notations

Although the general context of the present study is that of the automatic adaptive quadrature, the following discussion is limited to *local data*, derived on a single integration range. There is at least one good reason for such an approach: *the occasional failures* of the local error estimates which are overridden by decisions taken at the level of the general control routine are avoided in the reported statistics.

The present discussion is limited to GK 7-15 and GK 10-21 quadrature rules, the general description of which is given in QUADPACK [8]. With minor reformulation, the derived results hold true for other quadrature rules as well (reference [9] is particularly illuminating in this respect).

Let I denote the actual value of the integral to be solved numerically,

$$I = \int_a^b f(x)dx. \quad (1)$$

A subroutine which implements a Gauss-Kronrod quadrature rule for solving (1) provides at output a pair $\{r_K, e_K\}$. In the present context, r_K is the *computed approximation* of I by the Kronrod quadrature sum (4), while e_K is the *local error estimate* (15).

The GK quadrature uses a number of $2n + 1$ quadrature knots inside (a, b) ,

$$x_i = c + hy_i; \quad c = (b + a)/2; \quad h = (b - a)/2; \quad i = -n, -n + 1, \dots, n, \quad (2)$$

where the reduced quadrature knots y_i are defined on $[-1, 1]$, such that $y_0 = 0 < y_1 < y_2 < \dots < y_n < 1$, while $y_{-i} = -y_i$, $i = 1, \dots, n$. Symmetric quadrature weights $w_{-i} = w_i > 0$ are associated to the knots y_i .

The Gauss quadrature knots run over the subset of (2),

$$\{x_{i_G} \mid i_G = -n + 1, -n + 3, \dots, n - 1\}, \quad (3)$$

with associated symmetric quadrature weights $w_{-i_G} = w_{i_G} > 0$.

The Kronrod quadrature sum is given by

$$r_K \equiv Q_K[f] = \sum_{i=-n}^n w_i f(x_i). \quad (4)$$

The Gauss quadrature sum provides a lower degree approximation to I ,

$$r_G \equiv Q_G[f] = \sum_{i_G=-n+1}^{n-1} w_{i_G} f(x_{i_G}). \quad (5)$$

Then the local Ggk error estimate is given by

$$e_{ggk} = |r_K - r_G|. \quad (6)$$

Let $\tilde{f}$ denote the computed value of the average of $f(x)$ over $[a, b]$ at the knots (2),

$$\tilde{f} = r_K / (b - a), \quad (7)$$

and Δ denote the computed value of the integral $\int_a^b |f(x) - \tilde{f}| dx$, which measures the area covered by the deviations of $f(x)$ around $\tilde{f}$,

$$\Delta = Q_K [|f - \tilde{f}|]. \quad (8)$$

The local QDP error estimate is then given by

$$e_{qdp} = \Delta \times \min\{(200e_{ggk}/\Delta)^{3/2}, 1\}. \quad (9)$$

The values (6) and (9) are taken for error estimates provided they do not fall below the attainable accuracy limit imposed by the relative machine precision. The latter threshold is defined as the product

$$e_{roff} = \tau_0 \epsilon_0 Q_K [|f|]. \quad (10)$$

Here τ_0 is an empirical multiplicative factor (following QUADPACK, we have chosen $\tau_0 = 50$) and ϵ_0 denotes the relative machine accuracy.

For the case study integrals considered below, the value I of (1) is computed from the existing analytical expressions, such that the exact quadrature error e_Q of the numerical output r_K can be defined,

$$e_Q = I - r_K. \quad (11)$$

In the graphical presentation of the quadrature errors, the *moduli of the relative errors* (simply called relative errors in the sequel) are useful,

$$\varepsilon_\alpha = |e_\alpha / I|, \quad \alpha \in \{ggk, qdp, Q\}. \quad (12)$$

An error estimate $e_\alpha, \alpha \in \{ggk, qdp\}$ is said to be *reliable* provided that $|e_Q| \leq e_\alpha$, or equivalently,

$$\varepsilon_Q \leq \varepsilon_\alpha. \quad (13)$$

Within a subroutine which implements a quadrature rule, the derivation of the local error estimate, e_K , uses information inferred from the *estimated relative errors*,

$$\rho_\alpha = |e_\alpha / r_K|, \quad \alpha \in \{ggk, qdp\}. \quad (14)$$

3 Main results

The present study shows that an analysis of some key features of the integrand, done within the subroutine which implements the quadrature rule of interest, provides significant hints on the reliability of the local error estimate.

In the case of GK 7-15 and GK 10-21 quadrature rules, a local error estimate *self-validates itself* according to the following scheme:

$$e_K = \begin{cases} \max[e_{\text{roff}}, \min(e_{ggk}, e_{qdp})] & \text{iff reliability conditions fulfilled} \\ e_{qdp} \text{ \& error flag} & \text{otherwise} \end{cases} \quad (15)$$

When a self-validating quadrature rule is incorporated in an automatic adaptive quadrature program, substantial increase of the correctness of the automatic decisions is obtained for difficult integrands.

The reliability conditions entering Eq. (15) have been derived by the use of Eratosthenes' sieve method to the analysis of sets of data obtained over families of elementary integrals. This allowed us to identify characteristic trends of the error behaviour with the integrand variation and to formulate rules of thumb in agreement with the general theory of the Riemann integral.

If the computation results in a value $|r_K|$ exceeding the machine underflow, the error estimates e_{qdp} and e_{ggk} may be taken for reliable provided that

$$\rho_{qdp} < \tau_{qdp} \phi_d, \quad \tau_{qdp} = 0.5, \quad (16)$$

and respectively

$$\rho_{ggk} < \tau_{ggk} \phi_d, \quad \tau_{ggk} = 0.005. \quad (17)$$

(Under vanishingly small $|r_K|$, the conditions (16) and (17) are imposed on the absolute errors e_{qdp} and e_{ggk} respectively.)

Here, the constants τ_{qdp} and τ_{ggk} simply trace the line between error estimates carrying significant figures at output and error estimates which do not carry out any significant figure under the integration of *continuous monotonic integrands*. They refine the similar proposal made in [10] in a different case study integral.

The discouraging factor ϕ_d ,

$$\phi_d = 10^{\min(\lambda, \mu, \nu)} \leq 1, \quad (18)$$

is a quantity inferred from the analysis of the integrand structure. It secures sharper reliability thresholds in the case of *continuous non-monotonic integrands*.

The quantities λ and μ measure the consistency of the integrand profile inferred from its values at the Gauss and Kronrod abscissas respectively:

- Let i_{xg} and i_{xk} denote the number of the local extrema of the integrand inside (a, b) , which occur over the manifolds of integrand values at the Gauss and Kronrod abscissas respectively. Then

$$\lambda = i_{xg} - i_{xk} \leq 0. \quad (19)$$

- Let i_{zg} and i_{zk} denote the number of the intersections of the computed average value (7) of the integrand with the polynomials which interpolate $f(x)$ at the Gauss and Kronrod abscissas respectively. We have

$$\mu = i_{zg} - i_{zk} \leq 0. \quad (20)$$

The quantity ν provides a measure to the asymmetry of the distribution of the interpolatory polynomial values at the quadrature abscissas (2) around the computed average (7). Let i_{pk} and i_{mk} , respectively, denote the number of the i_{xk} extrema laying above and below $\tilde{f}$. Then

$$\nu = -|i_{pk} - i_{mk}| \leq 0. \quad (21)$$

4 Monotonic integrands

Figure 1: Relative errors of the GK 7-15 outputs for the family of integrals (22) at low and moderately large exponents n .

In this section we consider two families of elementary integrals:

- Integrals over $[0, 1]$ of the terms of the fundamental power series, x^n ,

$$\int_0^1 x^n dx = \frac{1}{n+1}, \quad n = 0, 1, \dots, 1023. \quad (22)$$

- Integration of a constant integrand (which simulates a centrifugal potential at large x) over ranges of variable length,

$$\int_0^b \frac{1}{x^2 + 1} dx = \arctan(b), \quad b = 2^n, \quad n = 0, 1, \dots, 511. \quad (23)$$

Figure 2: Same as fig. 1, for GK 10-21 outputs.

The solutions of the integrals (22) by GK 7-15 and GK 10-21 quadrature rules yielded specific dependences of the quadrature errors on the exponent n . The obtained data on the relative errors (12) and on the estimated relative errors (14) can be conveniently divided in two classes.

The first class covers the range of low and moderately large exponents n (figures 1 and 2). The low n end corresponds to reliable highly accurate solutions provided by the GK quadrature rules. The inferences emerging from the pairs of relative errors $\{\varepsilon_{ggk}, \rho_{ggk}\}$ and $\{\varepsilon_{qdp}, \rho_{qdp}\}$ are consistent with each other and with the usual evidence available on this subject.

The second class covers the large and asymptotically large exponents n (figures 3 and 4). Here, the cusps occurring in the ε_Q curves (at $n_t = 250$ within GK 7-15 quadrature and at $n_t = 499$ within GK 10-21 quadrature) come from the sign change of the exact errors e_Q (11) under the variation of n .

The family (23) illustrates a class of integrals involving a smooth monotonic integrand and integration domains of different lengths.

The most interesting features of the GK 7-15 and GK 10-21 quadrature rule solution dependences on the integration domain length are plotted in figures 5 and 6 respectively. Similar to figures 3 and 4, the apparent irregularities which can be noticed in the ε_Q data originate in the sign change of the exact errors e_Q (11) under the variation of the upper integration end.

Reliable GK solutions are obtained at low n exponent values, i.e., at small lengths of the integration intervals. Here, the inferences from the estimated relative errors ρ_α , Eq. (14), are in

Figure 3: Relative errors of the GK 7-15 outputs for the family of integrals (22) at exponents n running over the machine range.

good agreement with those from the corresponding relative errors ε_α , Eq. (12).

At the highest n values quoted in Eq. (23), however, the discrepancy between these two kinds of errors reaches 150 orders of magnitude, a feature which points to the well-known bad failure of both GK 7-15 and GK 10-21 quadrature rules for these integrals.

At asymptotically large exponents, $n > n_t$, in figures 3 and 4, and at the high n end ($n > 12$) of the plots in figures 5 and 6, the behaviour of the data can be summarized as follows:

- The ratio e_{ggk}/e_{qdp} of the quadrature errors computed at a same n is *independent* of n (while depending on the integrand and on the quadrature rule: it equals roughly 0.5 for both GK solutions of (22), while for the integrals (23), the GK 7-15 ratio equals 0.453 and the GK 10-21 ratio equals 0.443). This induces the occurrence of *equally spaced lines* associated to the pairs $\{\varepsilon_{ggk}, \varepsilon_{qdp}\}$ and $\{\rho_{ggk}, \rho_{qdp}\}$ respectively.
- The relative errors ε_{ggk} and ε_{qdp} decrease with the increase of n .

For the integrals (22) and GK 7-15 quadrature, the decreasing ε_{ggk} and ε_{qdp} values fall below the ε_Q values at $n \geq 621$ and $n \geq 762$ respectively, where the validation criterion (13) is *not fulfilled*.

For the integrals (23), both relative errors ε_{ggk} and ε_{qdp} fall below ε_Q , with a *noticeable negative linear slope*.

Figure 4: Same as fig. 3, for GK 10–21 quadrature rules.

- In contradistinction to the relative errors ϵ_{ggk} and ϵ_{qdp} , the estimated relative errors (14) of both quadrature rules remain *constant* with n and above ϵ_Q , except for the ρ_{ggk} values within the family (23).

In view of the increased reliability of the QDP error estimator, the derivation of quantitative criteria intended to enhance output confidence naturally starts with the ρ_{qdp} data. Figures 1 to 6 show that, for both families of integrals and both quadrature rules, the validation condition (16) with $\phi_d = 1$ simply separates the QDP error estimates which carry at least one significant figure at output from those which do not carry any significant figure.

Within the automatic adaptive quadrature, an estimated QDP relative error worse than 50% points to a too crude approximation of the integral over the current subrange. In that case, the return of an *error flag* will unambiguously tell to the control routine of the automatic adaptive quadrature that the current integration range needs further subdivision.

Case study integrals of smooth integrands of interest in physics considered in [10, 11] illustrated the usefulness of such a criterion as a measure to prevent inappropriate activation of an extrapolation algorithm thought to accelerate the convergence.

Inspection of the data in figures 1, 2, 5, and 6 evidences the occurrence of a remarkable coincidence between the threshold associated to the significant ϵ_{qdp} errors and the level of *two significant figure accuracy* predicted by the GGK error estimate ϵ_{ggk} .

Let us assume that the two-figure accuracy of equation (17) with $\phi_d = 1$ is required as

Figure 5: Sample of the GK 7-15 relative errors (12) and (14) for the integrals (23). The values n on the abscissa axis specify the integration domain length $b = 2^n$.

a significance condition for the e_{ggk} error estimate, together with the return of an error flag under its infringement. For the families of integrals (22) and (23), this would simply mean an equivalent way of specifying the self-validation test of the local error estimate.

Under the fulfilment of both criteria, the QDP error estimate (9) will sharpen the precision under an accurate r_K approximation of the integral (1), while the GGK error estimate (6) will sharpen the error estimate under reliable but less accurate r_K . The motivation for the proposal (15) of defining the error estimate is thus completed.

This scheme results in a striking similarity to the three-region integrand behaviour (strong asymptotic, weak asymptotic, non-asymptotic) proposed in [9] on a quite different ground.

5 Non-monotonic integrands

In this section we consider the following families of test integrals:

$$(C1) \quad \int_{-1}^1 e^{p(x-x_0)} \cos(\omega x) dx = \quad (24)$$

$$(C2) \quad \int_0^1 2e^{-px_0} \cosh(px) \cos(\omega x) dx = \quad (25)$$

$$= 2e^{-px_0} [p \sinh(p) \cos(\omega) + \omega \cosh(p) \sin(\omega)] / (\omega^2 + p^2); \quad (26)$$

$$(S1) \quad \int_{-1}^1 e^{p(x-x_0)} \sin(\omega x) dx = \quad (27)$$

Figure 6: Same as fig. 5, for GK 10-21 quadrature rules.

$$(S2) \quad \int_0^1 2e^{-px_0} \sinh(px) \sin(\omega x) dx = \quad (28)$$

$$= 2e^{-px_0} [p \cosh(p) \sin(\omega) - \omega \sinh(p) \cos(\omega)] / (\omega^2 + p^2). \quad (29)$$

The parameter ω was chosen to run over the set of values

$$\omega_n = n\pi/60, \quad n \in \{0, 6000\}, \quad (30)$$

the assigned values of the parameter p were

$$p_m \in \{1, 2, 5, 10, 100\}, \quad (31)$$

while $x_0 = -1$, such that the non-oscillating factors of the given integrands are not symmetric with respect to the centre of the integration domain.

A summary of the statistics obtained over these families of integrals is given in Tables 1 and 2, where the number of failures of several error estimators are reported (bare GKG, bare QDP, as well as their various enhancements with validating conditions).

While the pairs of integrals **C1** and **C2** on one side and **S1** and **S2** on the other side are algebraically equivalent, the numerically provided outputs are found to differ to a large extent as it concerns the reliability of the error estimates and the accuracy of the reliable outputs at a given pair (p, ω) .

The first line of Table 1 shows that the bare GKG error estimators of the two quadrature rules are particularly unreliable for these kinds of integrals (with average rates of failure of 44.7%

Table 1: Reliability of various validation conditions^{(1),(2)}

Integrator	GK 7-15				GK 10-21			
Integrals	C1	C2	S1	S2	C1	C2	S1	S2
Bare G GK	2850	2599	2750	2534	2490	2257	2777	2285
Bare Q DP	433	258	25	168	254	115	33	61
τ_{qdp}	25	39	13	15	15	11	19	15
τ_{ggk}	14	18	13	18	21	12	18	15
$\tau_{qdp} \& \tau_{ggk}$	10	14	12	15	15	11	17	14
$10^\lambda \tau_{qdp}$	0	1	0	1	0	0	2	0
$10^\lambda \tau_{ggk}$	0	1	0	1	0	0	2	0
$10^\lambda \tau_{qdp} \& 10^\lambda \tau_{ggk}$	0	1	0	1	0	0	2	0
$10^\mu \tau_{qdp}$	1	1	1	5	0	0	2	3
$10^\mu \tau_{ggk}$	2	1	1	6	2	0	1	2
$10^\mu \tau_{qdp} \& 10^\mu \tau_{ggk}$	1	1	1	5	0	0	1	2
$10^m \tau_{qdp}^{(3)}$	0	0	0	1	0	0	1	0
$10^m \tau_{ggk}$	0	0	0	1	0	0	0	0
$10^m \tau_{qdp} \& 10^m \tau_{ggk}$	0	0	0	1	0	0	0	0

⁽¹⁾The integrals (24), (25), (27), (28): $p = 1$; ω runs over the set of 6000 values (30).

⁽²⁾Number of spurious error estimates out of 6000 test integrals on each column.

⁽³⁾ $m = \min(\lambda, \mu)$, with λ and μ defined by Eqs. (19) and (20) respectively.

and 40.9% of the GK 7-15 and the GK 10-21 error estimators respectively). The data in the second line of Table 1 shows that the rates of failures of the bare QDP error estimators are substantially lower than those of the corresponding G GK error estimators (the figures are roughly 3.7% and 1.9% respectively).

Table 1 seems to suggest that the G GK error estimators are particularly sensitive to the *length of the integration interval* [the GK 7-15 and GK 10-21 figures are 46.7% and 42.8% respectively over the set of families of integrals (24) and (27), while 43.9% and 37.9% over the set of families of integrals (25) and (28)].

As it concerns the QDP error estimators, Table 1 suggests that the *nature of the weight function* is important [the GK 7-15 and GK 10-21 figures are 5.8% and 3.1% respectively over the set of families of integrals (24) and (25), as compared to 1.6% and 0.8% over the set of families of integrals (27) and (28)]. The data in Table 2 go along the same pattern at $p = 2$ as well. However, at higher p values, the distribution of the spurious errors over the various families of integrals is substantially modified. An obvious specific pattern of the distribution of the failures of the two kinds of local error estimators is therefore absent.

The reliability secured by the validation conditions (16) and (17), at parameter values ($\tau_{qdp} = 0.5$, $\tau_{ggk} = 0.005$, and $\phi_d = 1$) fixed by the analysis done in the case of monotonic integrands, is reported in the third to fifth lines of Table 1. The number of spurious error estimates validated by *each of these conditions* is substantially lower than the corresponding figures occurring under

Table 2: (p, ω) dependence of reliability of validation conditions^{(1),(2)}

	Integrator	GK 7-15				GK 10-21			
p	Integrals	C1	C2	S1	S2	C1	C2	S1	S2
1	Bare QDP	433	258	25	168	254	115	33	61
	$10^m \tau_{qdp} \& 10^m \tau_{ggk}^{(3)}$	0	0	0	1	0	0	0	0
	$\tau_{qdp} \phi_d \& \tau_{ggk} \phi_d$	0	0	0	0	0	0	0	0
2	Bare QDP	154	218	23	115	17	96	32	27
	$10^m \tau_{qdp} \& 10^m \tau_{ggk}$	2	1	0	0	0	0	2	0
	$\tau_{qdp} \phi_d \& \tau_{ggk} \phi_d$	0	0	0	0	0	0	0	0
5	Bare QDP	24	40	27	28	11	20	29	27
	$10^m \tau_{qdp} \& 10^m \tau_{ggk}$	0	0	1	1	1	0	1	0
	$\tau_{qdp} \phi_d \& \tau_{ggk} \phi_d$	0	0	0	0	0	0	0	0
10	Bare QDP	67	23	74	17	38	17	37	24
	$10^m \tau_{qdp} \& 10^m \tau_{ggk}$	31	0	16	2	4	0	7	2
	$\tau_{qdp} \phi_d \& \tau_{ggk} \phi_d$	0	0	0	0	0	0	0	0
100	Bare QDP	327	60	320	59	58	64	54	60
	$10^m \tau_{qdp} \& 10^m \tau_{ggk}$	0	0	0	0	1	0	1	0
	$\tau_{qdp} \phi_d \& \tau_{ggk} \phi_d$	0	0	0	0	0	0	0	0

⁽¹⁾The integrals (24), (25), (27), (28): ω runs over the set of 6000 values (30).

⁽²⁾Number of spurious error estimates out of 6000 test integrals on each column.

⁽³⁾ $m = \min(\lambda, \mu)$, with λ and μ defined by Eqs. (19) and (20) respectively.

the bare QDP error estimators. The substantial improvement of output reliability which follows from these validation conditions have been found to hold true for the other investigated p values as well.

There are two features of the validation conditions (16) and (17) which are worth noting. First, when one of them is associated to a *severe failure* of the validation condition (13), the other one fails to detect the occurrence of a spurious output. Second, there is a very high degree of overlap between the sets of wrong output diagnostics issued by the two conditions over a given family of integrals.

These features allow us to infer that the remaining wrong diagnostics should have a common origin. The study of the integrand profile following from its values at the full set of quadrature knots (2) and at the Gauss subset (3) showed that further improvement of the error diagnostics can be obtained by imposing the natural validation condition of *consistency of the integrand profiles following from the two sets of data*.

The question arises, of course, how should this consistency be characterized quantitatively. The *number of local extrema* over the two sets of points and the *number of intersections of the two interpolatory polynomials with the integrand average over $[a, b]$* , Eq. (7), provide simple answers to this problem, with a small additional computing effort only.

Once these quantities are defined, the next problem is how to implement the obtained infor-

Figure 7: Self-validated error estimates (15) returned by the GK 7-15 and GK 10-21 quadrature rules for the family of integrals (24) at $p = 1$. Here and in the following figures, the subscript 15 refers to GK 7-15 quadrature outputs, while the subscript 21 refers to GK 10-21 quadrature outputs. The vertical lines delimit ends of ω values inbetween which self-validated errors (15) are returned.

mation as a validation condition. We found that the sharpening of the validation conditions (16) and (17) with a *discouraging factor* ϕ_d , Eq. (18) provides a convenient way of incorporating this supplementary information.

Table 1 illustrates the separate and combined effects of these two sharpening validation conditions. The figures in the **C2** and **S1** columns show that, as a rule, the two filters of error validation are *not* corroborated with each other, such that their combined effect results in enhanced output reliability.

Table 2 shows that the validation criterion based on the consistency of the profiles emerging from the Gauss subset and the full Kronrod set of integrand values still allows spurious error diagnostics. A particularly large number of failures occurs in the case $p = 10$. At large p values, all the failures happened under sharp integrand increase at one of the integration ends, resulting in a highly asymmetric distribution of the integrand values with respect to the average value (7). The validation parameter ν , Eq. (21), is intended to discourage the validation of the outputs characterized by such asymmetric distributions.

The last lines at each p value in Table 2 show that the addition of the last validation condition decreased the number of spurious error estimates down to zero. The natural question which arises at this point is the price paid to achieve this 100% reliability. Figures 7 to 12

Figure 8: Same as fig. 7, for the family of integrals (25).

provide an excerpt from the obtained outputs.

In each of these figures, comparisons of the exact relative errors (denoted ε_{15} for GK 7-15 quadrature and ε_{21} for GK 10-21 quadrature) with the *self-validated estimated errors* ρ_{15} and ρ_{21} respectively are given for various values of the parameter p .

The occurrence of lower accuracies of both the estimated and exact relative errors at ω values lying in the neighbourhood of multiples of π [in the case of the integrals (24) and (25)] and of odd multiples of $\pi/2$ [in the case of the integrals (27) and (28)] stems from the loss of significant figures by subtraction. Similar to figures 3 and 4, the cusps pointing towards the minima of the exact relative errors originate in sign changes of the errors e_Q (11) under the variation of ω .

The plots in figures 7 and 8, with integrands characterized by a moderate variation of the non-periodic factors over the integration range, show that both quadrature rules reach the machine accuracy at the low ω end. This feature simply shows that both the Gauss and Kronrod approximations, Eqs. (4) and (5), solve the integrals to machine accuracy. However, the round-off threshold ceases to be simply a plateau as in the case of the polynomial integrals (22). Under GK 10-21 quadrature, three out of the four families of integrals (**C1**, **C2**, and **S2**) show the occurrence of a round-off bottom sharply modulated by the cancellation by subtraction. In the case of the less accurate GK 7-15 quadrature, the modulation was present within the **C2** family of integrals only. Under $p = 1$, a round-off bottom is present in all cases. At $p \geq 2$, it disappears under the GK 7-15 quadrature. When present, its extension is more than double in the **C2** and

Figure 9: Self-validated error estimates (15) returned by the GK 7-15 and GK 10-21 quadrature rules for the family of integrals (24) at $p = 2$.

S2 integrals as compared to their **C1** and **S1** counterparts.

In each case, the sharpest of the QDP estimates (9) and the Ggk estimates (6) are taken for the error estimates. Thus, above the round-off bottom, the error estimate e_K , Eq. (15), equals e_{qdp} , Eq. (9), towards the higher accuracy side and it equals e_{ggk} , Eq. (6), towards the lower accuracy side.

A look at figures 7 to 12 shows that the threshold $\tau_{ggk} = 0.005$ established in the case of monotonic integrands, is rarely reached. Usually, the local error estimates, the values of which stay within a few orders of magnitude below this threshold, are ruled out due to the occurrence of values of the discouraging factor (18) smaller than unity. It happens that the overwhelming part of the chopping comes from the asymmetry factor (21) of the interpolatory polynomial.

Figures 11 and 12 provide samples of GK 10-21 outputs obtained under large variations of the non-oscillatory part of the integrand over the integration domain. At $p = 5$, the round-off bottom disappears in the case of the **C1** and **S1** families of integrals. Finally, at $p = 10$, it is absent in the other two families of integrals, **C2** and **S2** as well, a feature which tells us that the Gauss polynomial (5) cannot solve these integrals to machine accuracy. As a rule, the chopping operated by the validation conditions (16) and (17) increases with the magnitude of the integrand variation over the integration domain $[a, b]$. As a consequence, the range of ω values over which a reliable quadrature output is reached in a single step (i.e., without needing subrange subdivision) drastically shrinks with the increase of p (at $p = 100$, except for $\omega = 0$

Figure 10: Same as fig. 9, for the family of integrals (25).

under **S1** and **S2** integrals, all the returned outputs pointed towards the absence of reliable significant figures in r_K).

6 Comments and conclusions

The present study started from the need to get reliable numerical solutions of some difficult integrals occurring in a gauge theory model of cuprate superconductors [2, 3]. An important prerequisite to be satisfied by the automatic quadrature algorithm was the substantial increase of the reliability of the local error estimates. We have found that Eratosthenes' sieve method can be successfully used to derive validation criteria which are *adapted to the integrand structure*.

Having in mind the physical model of interest, we considered several families of integrals both over monotonic integrands, Eqs. (22), (23), and non-monotonic integrands (24), (25), (27), (28). The range of variation of the discrete parameters entering the families of integrals over monotonic integrands was extended to the machine range. The considered discrete sets of values of the continuous parameters entering the families of non-monotonic integrands were chosen such as to exhaust the various conceivable practical instances.

We have found that the reliability of the local error estimates can be substantially enhanced by means of two validation criteria, Eqs. (16) and (17), the implementation of which in the appropriate subroutines requires only a small additional computing effort.

Two adverse properties of the self-validating local error estimator (15) can be noticed:

Figure 11: Self-validated error estimates (15) returned by the GK 10-21 quadrature rules for the families of integrals (24) and (25) at $p = 5$.

- When accepted by the validation conditions, the returned error estimate equals the *sharpest available error estimate*.
- The drop-off of the spurious coincidences resulting in apparently accurate local error estimates also removes most of the reliable error estimates the accuracy of which lies near the threshold τ_{ggk} , Eq. (17). Thus, the actual accepted level of accuracy of the error estimates gets substantially sharper in the case of non-monotonic integrands.

In view of their accessibility, we concentrated our efforts to the study of the reliability of local error estimates entering GK 7-15 and GK 10-21 quadrature rules [8]. The resulting subroutines will be submitted for publication in the CPC Library in the nearest future.

The ideas developed within the present approach can be extended to the analysis of other families of integrals as well. The obtained results might serve as preconditioners to alternative solutions of two kinds of problems where the heuristics is known to be important: the enhancement of the reliability of other local error estimates [9, 12], and the decision on the occurrence of a good starting point for the activation of an extrapolation algorithm [13].

Figure 12: Self-validated error estimates (15) returned by the GK 10-21 quadrature rules for the families of integrals (27) and (28) at $p = 10$.

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