Classes of integrals in the automatic adaptive quadrature

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Overview

- **General frame of the Bayesian automatic adaptive quadrature (BAAQ)**
- Three classes of integration domain lengths
- Reliability of accuracy specifications
- Improved diagnostic tools for Bayesian inference over macroscopic range lengths
- Conclusions

General frame (1)

The high performance computing in physics research frequently asks for fast and reliable computation of Riemann integrals as part of the models involving evaluation of physical observables.

A numerical solution of the Riemann integral

$$I \equiv I[f] = \int_a^b g(x)f(x)dx, \qquad -\infty \leq a < b \leq \infty,$$

is sought under the assumption that the real valued ***integrand function*** $f(x)$ is continuous almost everywhere on $[a, b]$ such that I exists and is finite.

The ***weight function*** $g(x)$ either absorbs an analytically integrable difficult factor in the integrand (e.g., endpoint singularity or oscillatory function), or else $g(x) \equiv 1,\ \forall\, x \in [a, b]$.

General frame (2)

The automatic adaptive quadrature (AAQ) solution of I provides an approximations $Q \equiv Q[f]$ to $I[f]$ based on ***interpolatory quadrature***.

The ***meaningfulness*** of the output $Q[f]$ is assessed by deriving a **bound** $E \equiv E[f]$>0 to the **remainder** $R[f] = I[f] - Q[f]$.

For a prescribed accuracy τ ***requested at input***, the approximation Q to I is assumed to **end the computation** provided

$$|R[f]| < E < \tau.$$

The definition of τ needs two parameters: the **absolute accuracy** ε_a and the **relative accuracy** ε_r , such that

$$\tau = \max\{\varepsilon_a,\ \varepsilon_r \cdot |I|\} \simeq \max\{\varepsilon_a,\ \varepsilon_r \cdot |Q|\}.$$

General frame (3)

If the condition of termination of the computation is not satisfied, the ***standard automatic adaptive quadrature*** (SAAQ) approach to the solution attempts at decreasing the error E by the ***subdivision*** of the integration domain $[a, b]$ ***into subranges*** using ***bisection*** and the computation of a ***local pair*** $\{q, e > 0\}$ over **each newly defined subrange** $[\alpha, \beta] \subset [a, b]$.

This procedure builds a ***subrange binary tree*** the evolution of which is controlled by an associated ***priority queue***.

Local pairs $\{q_i, e_i > 0\}$ are computed over the i-th subrange of $[a, b]$ and ***global*** outputs $\{Q_N, E_N > 0\}$ are got by summing the results obtained over the N existing subranges in $[a, b]$.

After each subrange binary tree update, the termination criterion is checked until it gets fulfilled.

General frame (4)

Within SAAQ, the derivation of ***practical bounds*** $e > 0$ to q rests on ***probabilistic arguments*** the validity of which is subject to doubt.

The BAAQ advancement to the solution incorporates the rich SAAQ accumulated empirical evidence into a general frame based on the ***Bayesian inference***. While the probabilistic derivation of practical bounds to the local quadrature errors is preserved, each step of the gradual advancement to the solution is scrutinized based on a set of ***hierarchically ordered*** criteria which enable decision taking in terms of the stability of the established Bayesian diagnostics.

The present report stresses two main things: (i) the need of using ***length scale dependent quadrature sums*** and (ii) the importance of the scrutiny of the ***range of variation of the generated integrand profile*** in order to decide on the use of a SAAQ-based approach to the solution or on the need of full use of the BAAQ analysis machinery.

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Symmetric Decomposition of the SAAQ Integrand Profiles

- For any $[\alpha,\beta]\subseteq[a,b]$ we write the ***symmetric*** decomposition
$$[\alpha,\beta]=[\alpha,\gamma]\cup[\gamma,\beta],\ \ \gamma=(\beta+\alpha)/2,\ h=(\beta-\alpha)/2.$$
- Over the ***left*** (l) and ***right*** (r) halves of $[\alpha, \beta]$, the floating point integrand values entering the quadrature sums are computed respectively as
$$f_k^l=f(\alpha+h\eta_k),\ \ f_k^r=f(\beta-h\eta_k),$$
where
$$0\le\eta_0<\eta_1<\cdots<\eta_k<\cdots\eta_n=1,\ \ n\in\{n_{\mathrm{CC}},n_{\mathrm{GK}}\}$$
stay for the floating point values of the ***reduced modified quadrature knots*** associated to either the Clenshaw-Curtis (CC) or the Gauss-Kronrod (GK) quadrature sums.
- Notice that $f_0^{\,l}=f(\alpha),\ f_n^{\,l}=f_n^{\,r}=f(\gamma),\ f_0^{\,r}=f(\beta)$ are ***inherited*** from ancestor subranges while at $0<\eta_k<1$, values $f_k^{\,l}, f_k^{\,r}$ are computed at ***each*** attempt to evaluate $I[\alpha, \beta]\,f$.
- **Definition.** The ***integrand profiles over half-subranges*** consist of appropriately chosen ***sets of pairs*** $\{\eta_k\,, f_k^{\,l}\}$ and $\{\eta_k\,, f_k^{\,r}\}$ respectively, including those coming from the abscissas pairs $\{\alpha, \gamma\}$ and $\{\gamma, \beta\}$.
- Other symmetric quadrature rules result in similarly defined integrand profiles.

Algebraic and Floating Point Degrees of Precision

• The ***algebraic degree of precision***, d, is an invariant feature of a quadrature sum over the field $\mathbb{R}$ of the real numbers: its value remains *constant* irrespective of the *extent* and the *localization* of the current integration domain over the real axis.

• Under floating point computations, the characterization of an interpolatory quadrature sum is made by its ***floating point degree of precision***, d_{fp}.

Given the integration domain $[a, b]$ $(a \neq b)$, the value of d_{fp} is determined by the magnitude of the parameter

$$\rho = |L| / \max\{1.0, X\}, \quad 0 < \rho \leq 2,$$

where

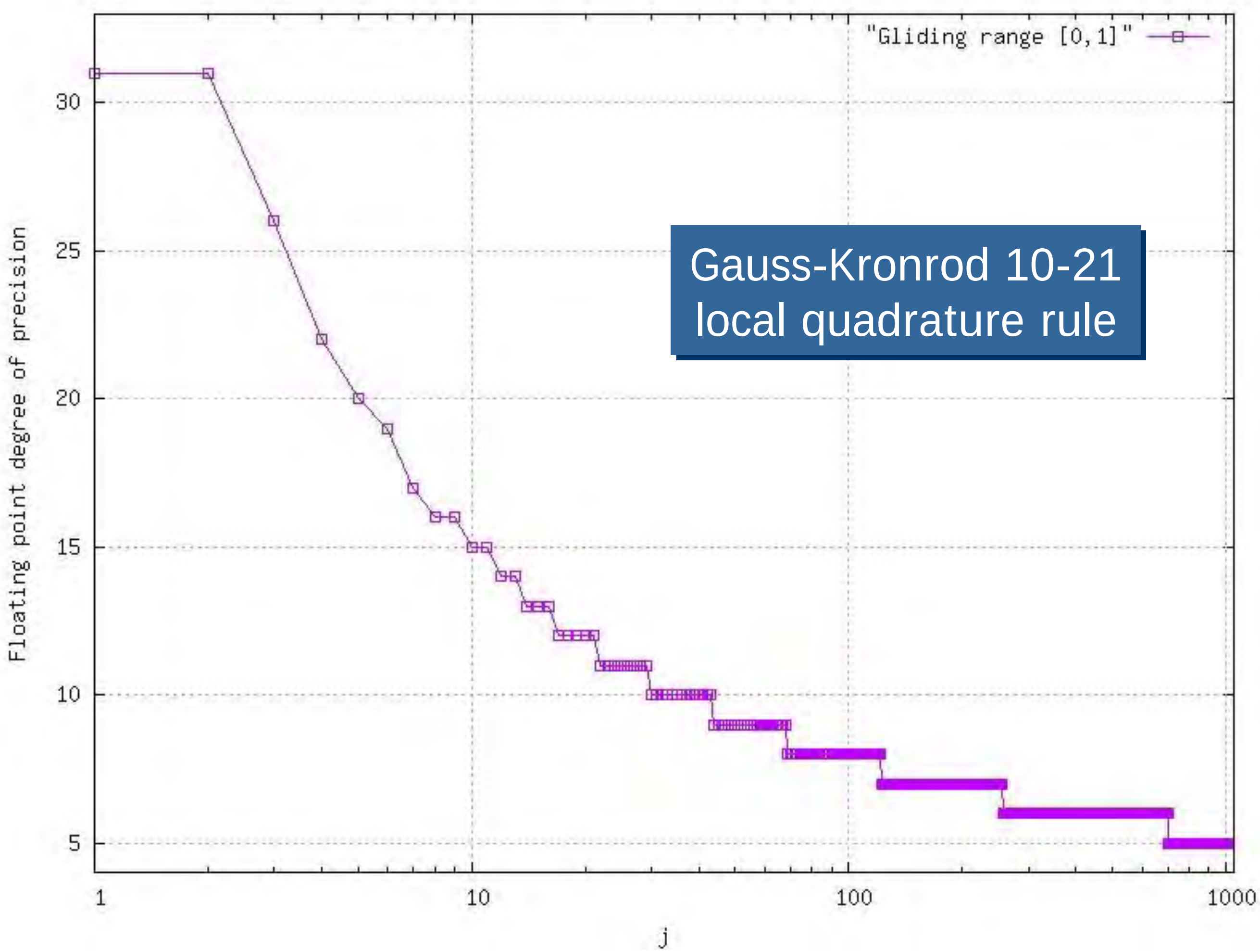
$$L = b - a \quad (L \neq 0.0); \quad X = \max\{|a|, |b|\} \quad (X > 0.0).$$

The quantity ρ defines the *floating point scale length* of $[a, b]$.

Features of the Floating Point Degree of Precision

- *Gliding integration range* [0,1] *on the real axis.*

The following plot gives outputs for the family of 1024 integration ranges $\{[j\alpha, j\alpha + \beta], \alpha = \beta = 1; j = 0, 1, \ldots, 1023\}$



Variation of the floating point degree of precision of the GK 10-21 local quadrature rule over the gliding range **[0, 1]** ***versus its distance j from the origin.*** It is shown that $d_{fp} = d = 31$ at low j values ($j = 0, 1, 2$), then d_{fp} abruptly decreases at larger but small enough j, to show slower decreasing rates under the displacement of [0,1] far away from the origin, reaching a bottom value $d_{fp} = 5$ at $701 \leq j \leq 1023$.

The Inverse Problem

- Find the family of the integration ranges $[\alpha, \beta]$ over which the floating point degree of precision cannot exceed a prescribed value d.
- Possibilities at hand:

 - $d = 2$ (the, perhaps composite, trapezoidal rule),
 - $d = 4$ (the, perhaps composite, Simpson rule),
 - $d \gg 1$ (the SAAQ used GK 10-21 or CC 32).

Each of these three cases corresponds to specific integration domain lengths, which are separated from each other by two empirically chosen thresholds, τ_μ and τ_m , defined below. They separate ***three classes of integration domain lengths*** corresponding to various quadrature sums at hand.

Three Classes of Finite Integration Domain Lengths

- ***Microscopic ranges*** [using (composite) ***trapezoidal rule*** ($d = 2$)], are characterized by the threshold condition

$$0 < \min(X,\ |L|/X) \leq \tau_\mu = 2^{-22}\ .$$

- ***Mesoscopic ranges*** [using (composite) ***Simpson rule*** ($d = 4$)], are characterized by the threshold condition

$$\tau_\mu = 2^{-22} < \min(X, |L|/X) \leq \tau_m = 2^{-8}\ .$$

- ***Macroscopic ranges*** [using ***quadrature sums of high algebraic degrees of precision***], are characterized by the threshold condition

$$\min(X, |L|/X) \leq \tau_m = 2^{-8}\ .$$

== $\boldsymbol{\tau_\mu = 2^{-22}}$ corresponds to ***d*** **= 3**

== $\boldsymbol{\tau_m = 2^{-8}}$ corresponds to ***d*** **= 8**; it results in **negligible round off** over the macroscopic domain lengths.

Exceptional Cases Ending Computation

- Irrespective of the domain scale, the **early Bayesian assessment** of the degree of difficulty of a given integral starts with the symmetrically decomposed integrand profile (IP) generated over the spanning modified reduced quadrature abscissas. A ***non-commutative decision chain results in the following diagnostics:***
- (i) ***The range of the* IP *variation*** enables the identification of a **constant integrand**.
- (ii) ***The measure of oddness of the* IP *distribution around its centre*** enables the identification of an **odd integrand**.
- (iii) ***Splitting the* IP *into subsets with interlacing abscissas*** and computation of quadrature sums by composite generalized centroid quadrature sums enables the identification of:
  - a **vanishing integral**;
  - occurrence of **catastrophic cancellation by subtraction**;
  - occurrence of an **easy integral**;
  - occurrence of a **difficult integral** asking for Bayesian analysis.

Asymptotic Tails

- If the reference Riemann integral is defined over an infinite domain, ($-\infty = a$ and/or $b = +\infty$) then there are two possibilities:
- (i) ***Mapping the infinite range onto*** [–1, 1]. This introduces a **singularity** at the endpoint corresponding to the infinite limit. Therefore, the use of an extrapolation procedure is compulsory.
- (ii) ***Replacing the infinite limit by a finite value***. The computation of the given integral over the resulting macroscopic finite range yields a finite reference value. Then the addition of a supplementary range toward the infinite limit allows the assessment of the **rate of decay** of the integrand at infinity.

  If the **integrand decays fast**, then computation can be stopped after a **small number of iterations**.

  If however, there is a **slow decay**, then a **Richardson extrapolation** improves the output.

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Input Reliability Check

- Let $\{\varepsilon_a^{(i)}, \varepsilon_r^{(i)}\}$ denote the values provided at input for the accuracy parameters.
- The input reliability check aims at setting up ***reliable*** values $\{\varepsilon_a^{(r)}, \varepsilon_r^{(r)}\}$ to be used within the BAAQ.
- $\varepsilon_a^{(i)}$ is mapped onto a non-negative value $\varepsilon_a^{(r)}$,

$$\varepsilon_a^{(r)} = \max\{\varepsilon_a^{(i)}, 0.0\}.$$

- $\varepsilon_r^{(i)}$ is mapped onto an inner value $\varepsilon_r^{(r)}$ satisfying

$$\varepsilon_r^{(r)} = \min\{rceil(), \max\{\varepsilon_r^{(i)}, rfloor()\}\};$$

$rceil() = 2^{-8}$; $rfloor() = 2^{-48}$ denote two empirically defined *environment functions*.

Integrand Dependent Accuracy Bounds

- After the solution of the **exceptional cases**, we remain with the pairs computed by the composite trapezoidal rule, $Q_N = Q_N[f]$ and $T_N = Q_N[|f|]$. Let $\rho_N = rfloor() \cdot (T_N / |Q_N|)$.
- The ***termination criterion is checked*** for ***integrand dependent accuracy bounds at output*** $\{\varepsilon_a^{(o)}, \varepsilon_r^{(o)}\}$,

$$|I - Q_N| < E_N < \max\{\varepsilon_a^{(o)}, \varepsilon_r^{(o)} |Q|\}.$$

Here $\varepsilon_a^{(o)} = \min\{\varepsilon_a^{(r)}, \max\{|Q_N|, 1.0\} \cdot rceil()\}$.

$\varepsilon_r^{(o)} = \max\{\varepsilon_r^{(r)}, \rho_N\}$, where $\{\varepsilon_a^{(r)}, \varepsilon_r^{(r)}\}$ denote the validated input.

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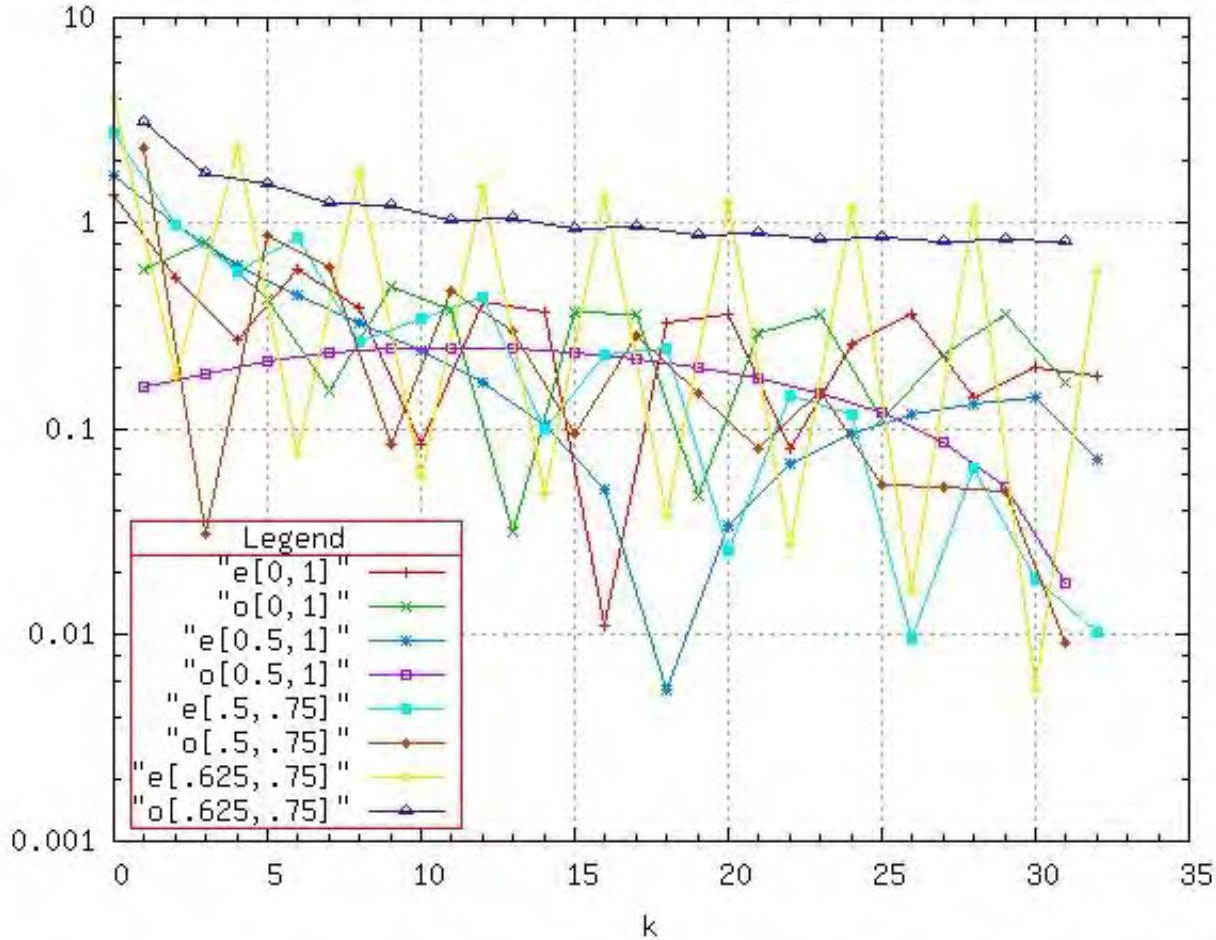
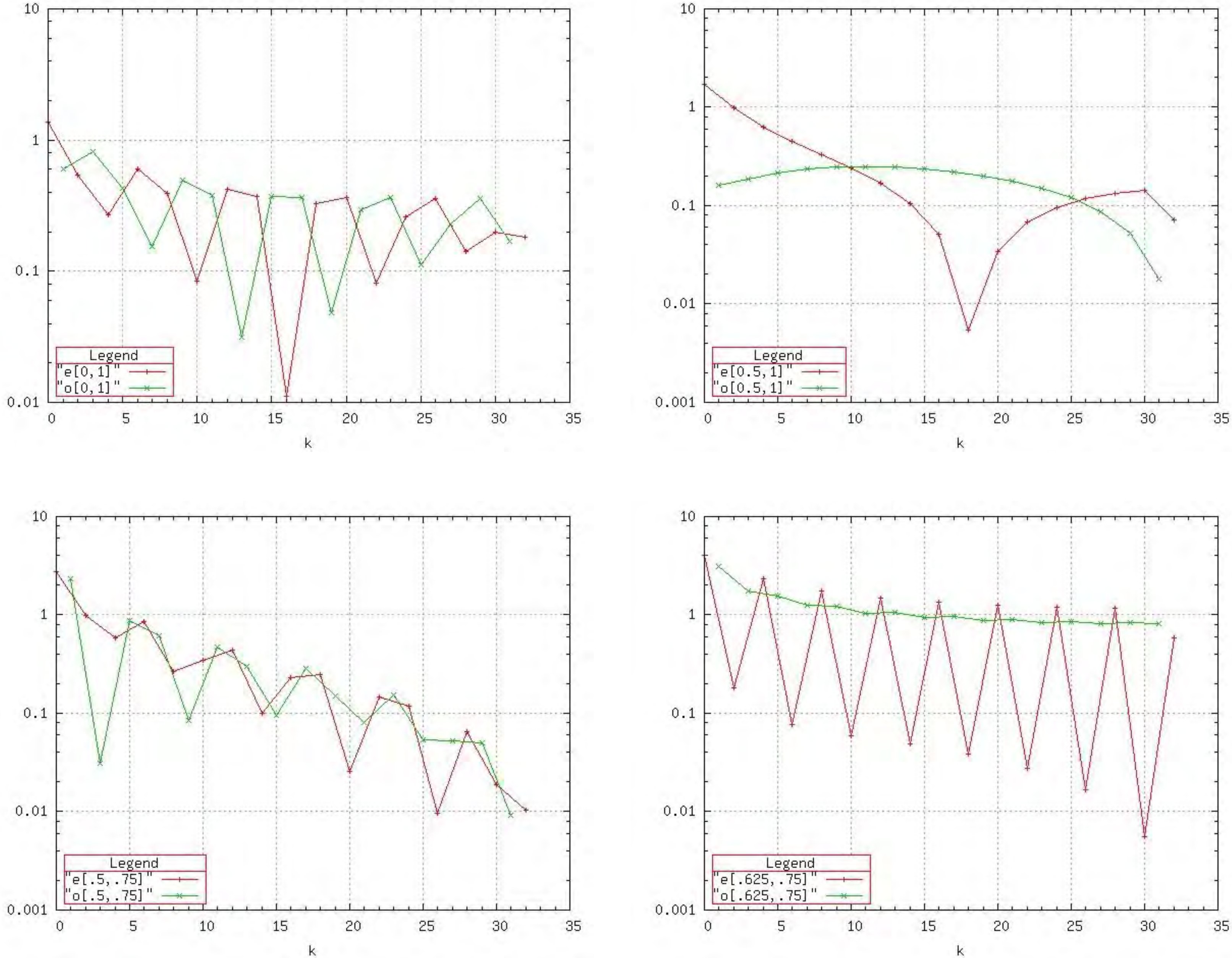
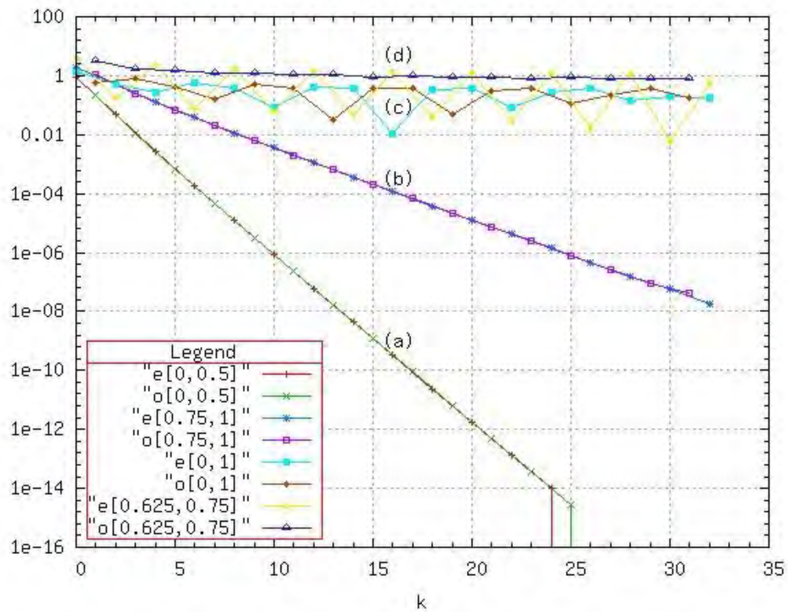


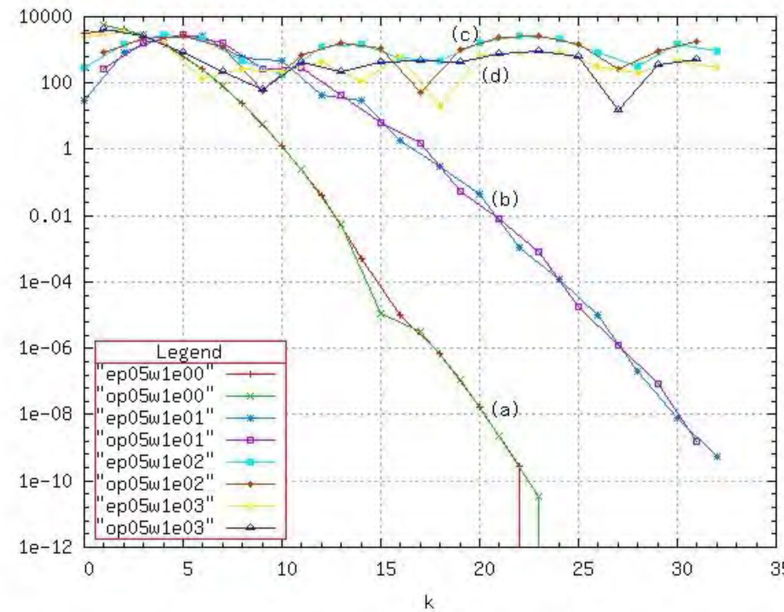
Ill-integrand behavior illustrated in the irregular variation of the Chebyshev expansion coefficients for the integrand $f_1(x) = |x^2 + 2x - 2|^{-1/2}: [0, 1] \to \mathbb{R}$ which shows an inner singularity at $x_s = \sqrt{3} - 1$ over the specified subranges. The file notations start with the specification of the rank of the Chebyshev subset: 'e' (for even) and 'o' (for odd).



10
1
0.1
0.01
0 5 10 15 20 25 30 35
k
Legend
"e[0,1]"
"o[0,1]"
10
1
0.1
0.01
0.001
0 5 10 15 20 25 30 35
k
Legend
"e[0.5,1]"
"o[0.5,1]"
10
1
0.1
0.01
0.001
0 5 10 15 20 25 30 35
k
Legend
"e[.5,.75]"
"o[.5,.75]"
10
1
0.1
0.01
0.001
0 5 10 15 20 25 30 35
k
Legend
"e[.625,.75]"
"o[.625,.75]"

Typical patterns of variation **of the absolute magnitudes of the Chebyshev expansion coefficients within the** ***even and odd rank subsets*** **versus the coefficient labels**





The data on the ***left figure*** were derived for the integrand $f_1(x) = |x^2 + 2x - 2|^{-1/2}\colon [0, 1] \to \mathbb{R}$ which shows ***an inner singularity*** at $x_s = \sqrt{3} - 1$ over the specified subranges.

The data on the ***right figure*** were derived for the family of integrand functions $f_2(x) = e^{p(x-x_0)} \sin(\omega x)\colon [-1, 1] \to \mathbb{R}$ in terms of the variable parameters p, x_0, and ω at $p = 5$ (marked as 'p05' in the file names), at fixed $x_0 = -1$ (not marked), and at the specified four ω values.

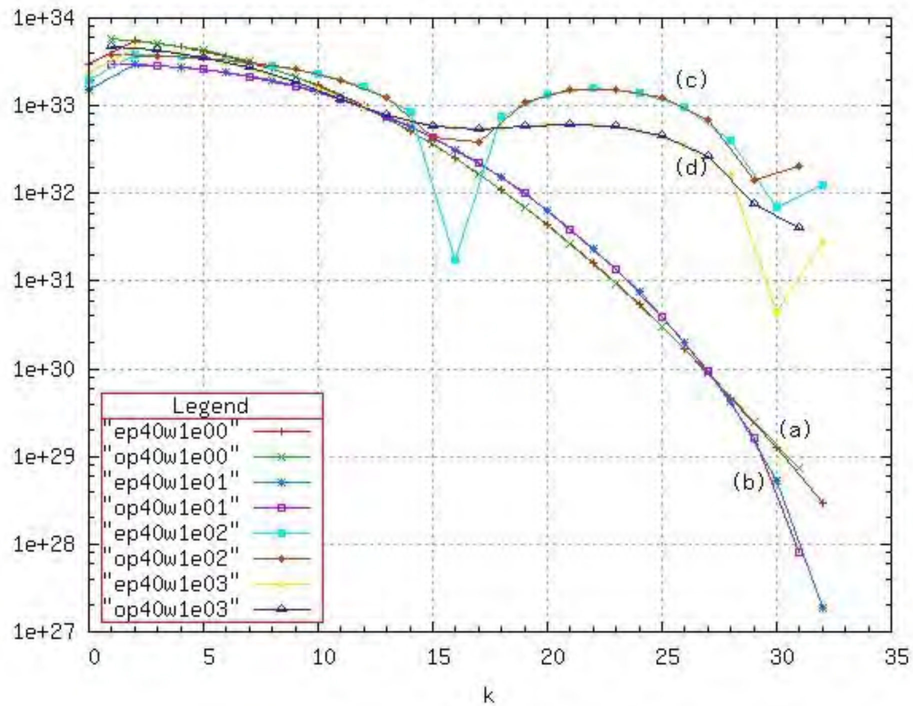
The file notations start with the specification of the rank of the Chebyshev subset: 'e' (for even) and 'o' (for odd).

Three typical integrand conditioning diagnostics are apparent:

(1) Cases (a): *well-conditioned, fast converging.*

(2) Cases (b): *well-conditioned, hopefully converging.*

(3) Cases (c) and (d): *ill-conditioned – integrand profile analysis requested to set precise diagnostic.*



The data were derived for the family of integrand functions $f_2(x) = e^{p(x-x_0)} \sin(\omega x) : [-1, 1] \to \mathbb{R}$ in terms of the variable parameters p, x_0, and ω at $p = 40$ (marked as 'p40' in the file names), at fixed $x_0 = -1$ (not marked), and at the specified four ω values.

The file notations start with the specification of the rank of the Chebyshev subset: 'e' (for even) and 'o' (for odd).

The same three typical integrand conditioning diagnostics are apparent:

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Conclusions (1)

• The identification of **exceptional cases** based on the analysis of the **range of variation of the integrand** is to start the Bayesian inference.

• The implementation of **termination criteria** using **integrand dependent** accuracy parameters enables the distinction between **easy integrals**, for which the SAAQ approach suffices and the **difficult integrals** for which the BAAQ approach is necessary.

• These results hold true and *avoid the overcomputing* provided three submanifolds of distinct integration domain ranges are selected, with specific quadrature sums:

- ***microscopic*** – *trapezoidal rule*,
- ***mesoscopic*** – *Simpson rule*, and
- ***macroscopic*** – *quadrature sums of high algebraic degrees of precision*

Conclusions (2)

• Over ***macroscopic integration ranges***, the **Clenshaw-Curtis** (CC) quadrature provides *fast and sensitive diagnostics*:

(i) *well-conditioned integrand*, typical for an easy (or hopefully converging) integral within the standard automatic adaptive quadrature approach;

(ii) *heavily oscillatory integrand* asking for the scrutiny of the possible redefinition of the attainable output accuracy within the BAAQ approach;

(iii) *highly probable integrand ill-conditioning* asking for the activation of the integrand profile analysis procedure for the inference of precise conditioning diagnostics.

Thank you for your attention !