Studies in Bayesian Automatic Adaptive Quadrature

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1. *A priori* Bayesian inference in numerical quadrature. The standard approach to the solution of one-dimensional Riemann integrals

$$I \equiv I_{ab}[f] = \int_a^b f(x)w(x)dx \ , \ -\infty < a < b < \infty, \tag{1}$$

within prescribed accuracy by automatic adaptive quadrature [1, 2], resulted in the implementation of computer codes (see, e.g., [1, 2, 3]) the reliability of which is heavily based on the user's ability to choose the suitable code from a menu of proposed automatic codes. While this approach constituted a big leap forward in numerical quadrature, the evidence shows that it may badly fail if a trial and error approach is needed due to the impossibility to know in advance the detailed behaviour of the integrand function (see, e.g., [4]).

Within the standard adaptive quadrature, the automatic decisions use as basic information the output pair $\{q, e\}$ of the *local quadrature rule* currently activated for solving $I_{\alpha\beta}[f]$ over a subrange $[\alpha, \beta] \subseteq [a, b]$. The automatic decisions will be correct under reliable $\{q, e\}$ pairs. However, spurious decisions with fatal outputs are possible under sequentially repeated occurrences of unreliable $\{q, e\}$ pairs.

Tools for the assessment of the $\{q, e\}$ pair reliability over the current integration range $[\alpha, \beta]$ have been proposed a few years ago [5, 6]. Essentially, they performed an *a posteriori* check of the well-conditioning of the *profile of the integrand function* $f(x)$, defined as the set of its values at the quadrature knots inside (α, β) together with the endpoint ones, $f(\alpha)$ and $f(\beta)$. At the ICCAM 2004 Conference we first proposed [7] the idea of *conditional activation* of the local quadrature rules. This had to be obtained by means of a set of hierarchically ordered *a priori* validation criteria providing *Bayesian inference* [8] on the well-conditioning of *gradually generated* integrand profile subsets at newly added quadrature knots.

The *root* of the Bayesian inference decision tree allowing ignition of the *integrand adapted activation* of a local quadrature rule for solving (1) concerns the *diagnostic of the behaviour of* $f(x)$ *at the boundaries* a *and* b *of the integration domain* $[a, b]$. The solution of this step of the Bayesian inference falls completely outside the standard pattern of the automatic adaptive quadrature. Its derivation from a suitable integrand sampling inside a *mesoscopic neighbourhood of the boundary layer* of $[a, b]$ is discussed in the following.

2. Mesoscopic analysis of the boundary layer. 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 nonvanishing neighbourhood $V(x_r) \subseteq [a, b]$ 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*, $\{f_i = fl(f(x_i)) | i = 0, 1, \cdots, m\}$, over a set of machine number arguments $S_m(x_r) = \{x_i \in V(x_r) | i = 0, 1, \cdots, m\}$, $m \geq 3$, chosen such that $fl(x_r) \in S_m(x_r)$, where $fl(\zeta)$ denotes the floating point representation of $\zeta \in \mathbf{R}$. Let $\{f(x_i)) | i = 0, 1, \cdots, m\}$ denote the set of *actual* values of $f(x_i)$ over $S_m(x_r)$. In general, due to the round-off, $f(x_i) - fl(f(x_i)) \neq 0$, hence the best information on the smoothness properties of $f(x)$ at x_r following from the

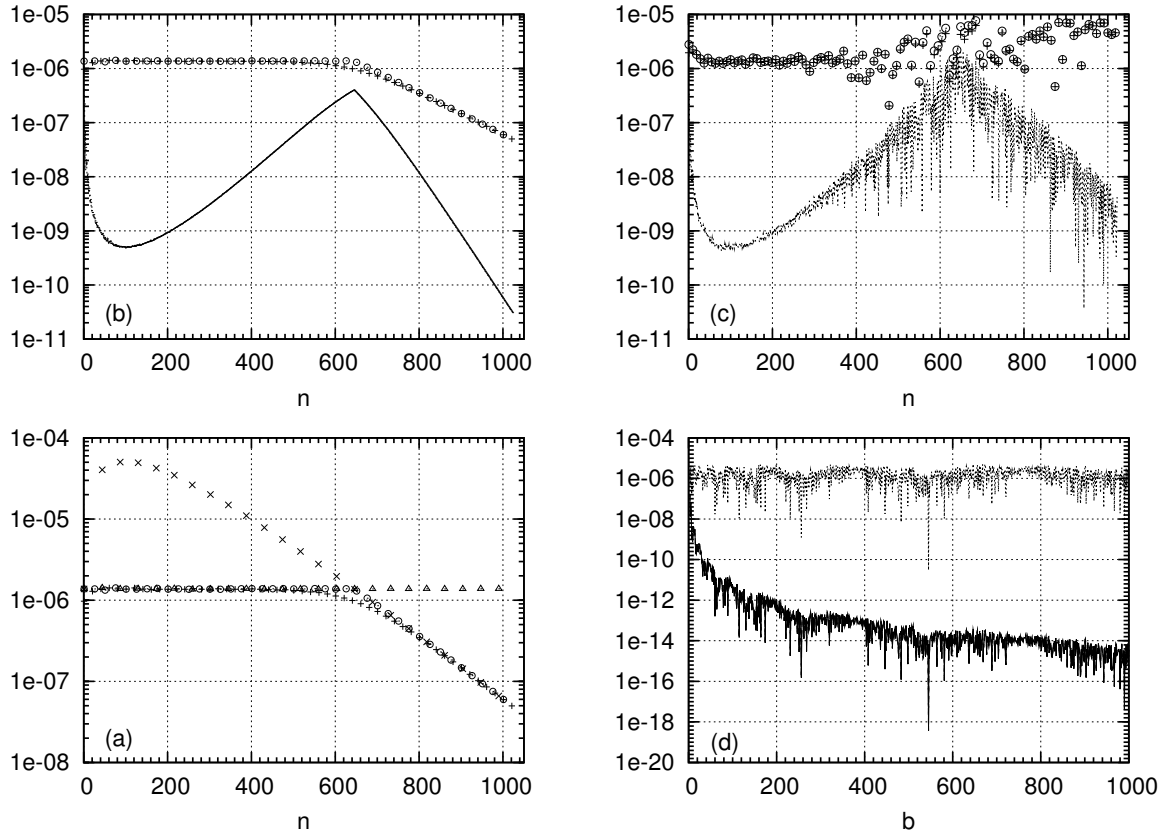

Figure 1: (a) Error measures of the first order derivative approximation (3) of $f(x) = x^n$, at $b = 0.99$ inside $[a, b] = [0.01, 0.99]$, in terms of the exponent values n. (b) Comparison of the affine and conventional error measures for the data on Fig. (a). (c) Same as (b) for $f(x) = x^n + 1$. (d) Same as (a) for $f(x) = 1/(1 + x^2)$, at b end inside $[0, b]$ for variable b. Within plot resolution, the affine, conventional and absolute error measures (lower graph) coincide with each other

set $\{x_i, f_i\}$ 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* $x_i = x_0 + \xi_i h_r,\ i = 0, 1, \cdots, m$, $\xi_i \in \mathbf{Z}$, 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

$$y_2(x_i) = \alpha_0 + \alpha_1 h_r p_1(\xi_i) + \alpha_2 h_r^2 p_2(\xi_i)\,, \tag{2}$$

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

$$f'(x_r) \approx y_2'(x_r) = \alpha_1 = N_1^{-1} \sum_{i=0}^{m} p_1(\xi_i) f_i. \tag{3}$$

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 chose 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 $f'(x)$.

3. Implementation of the analysis criteria. The extension of the analysis mesh $S_3(x_r)$ is subject to two contradictory requirements. If $f(x)$ is a *smooth slowly varying function*, then it is desirable to have an *as large as possible* mesoscopic sampling. Otherwise, it is desirable to have an *as narrow as possible* mesoscopic sampling. To conciliate these two requirements, we start with a trial value $1 \ll p \ll \varepsilon_0^{-1}$ (where ε_0 is the largest relative spacing between adjacent machine numbers) and compute f_0 and f_2. Under a large deviation of f_2 from f_0, the sampling abscissas x_1 and x_3 are chosen inside (x_0, x_2), while under a small deviation of f_2 from f_0, a value $q \gg p$ is used.

The analysis of the boundary layer yields, at each domain integration end:

(1) The diagnostic concerning the behaviour of the analyzed function: irregular behaviour inside the analysis neighbourhood; smooth function; inward monotonically decreasing function, pointing to the probable occurrence of a singularity in $f(x)$ or $f'(x)$, either at the analyzed domain end or at a nearby outer point, resulting in slow convergence; inward monotonically increasing function, pointing to the probable occurrence of an inner singularity in $f(x)$ or $f'(x)$, resulting in slow convergence.

(2) Under smooth function diagnostic, the estimate (3) of $f'(x_r)$ is returned.

(3) The number of function evaluations needed to infer the diagnostic associated to a boundary layer (that is, at both ends a and b of the analyzed interval) provides a measure to the efficiency of the proposed procedure.

The possibility of doing a *reliable and portable analysis* follows from the conformity of both the *hardware* (RAM, cache, processor) and the *software* (operating system and compiler) with the *IEEE 754 standard* [9] which governs binary floating point arithmetic.

While *checking software conformity with the IEEE 754 standard*, we identified and solved three points where the results of the straightforward implementation of the analysis were falsified: deviation of the *length of the significand* from the standard; *floating point comparison operation* deviations from the standard; unpredictable effects following from *compiler code optimization*.

We finally mention that the accuracy of the approximation of $f'(x_r)$ by $y_2'(x_r)$ was measured using both the conventional approach (which takes the minimum of the absolute and relative errors) and the unified affine measure proposed in [10].

4. Numerical results. The above analysis has been tested on several classes of parametric functions simulating various possible behaviours inside the boundary layer. The main conclusions of the analysis can be summarized as follows:

(i) *Robustness of the procedure:* Correct outputs have been obtained for function ranges going from the underflow threshold to the overflow threshold.

(ii) *Reliability of the procedure:* For all the investigated families of functions and all the considered sets of the parameters, the procedure resulted in truthful inferences.

(iii) *Output precision of first order derivative estimates:* For all the families of smooth functions, Eq. (3) yielded at least five exact significant decimal figures.

(iv) *Efficiency of the procedure:* The number of function evaluations needed for diagnostic inference varied from the minimal value of four to five.

Figures 1 and 2 summarize the most interesting results concerning the efficiency of derivative approximation by Eq. (3) in the case of continuous functions.

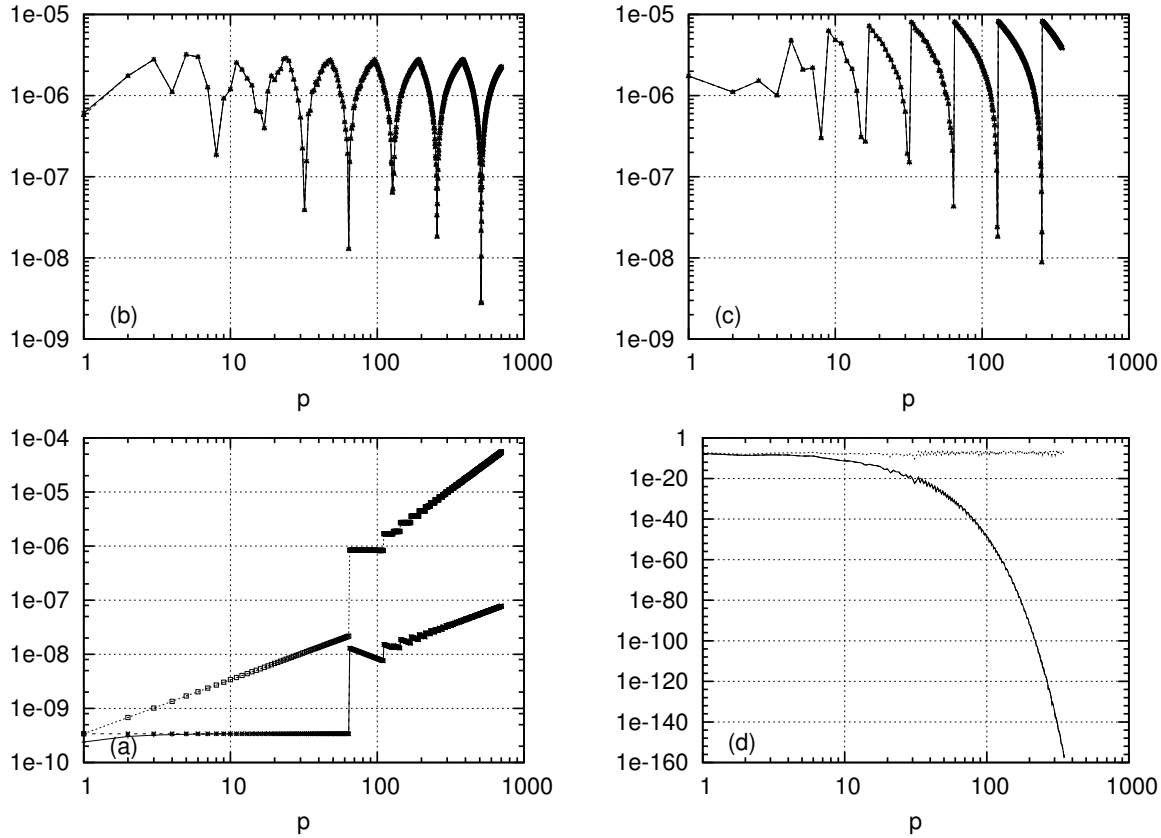

Figure 2: (a) Error measures associated to Eq. (3) for $f(x) = e^{px}$, at $a = 0$ inside $[a, b] = [0, 1]$ for variable p. The affine error deviates from the conventional and relative errors at low p. (b) Same as (a), at $b = 1$ end. The affine, conventional and relative errors are identical within plot resolution. (c) Same as (b), at $b = 1$ end for $f(x) = e^{p(x+1)}$. All mentioned errors are identical within plot resolution. (d) Same as (c), at $a = 0$ end for $f(x) = e^{p(x-1)}$. The precision is controlled by the absolute error, while the relative one mostly remains in the range $10^{-8} \div 10^{-7}$

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