An Overview of the Numerical Solution of Gauge Integrals

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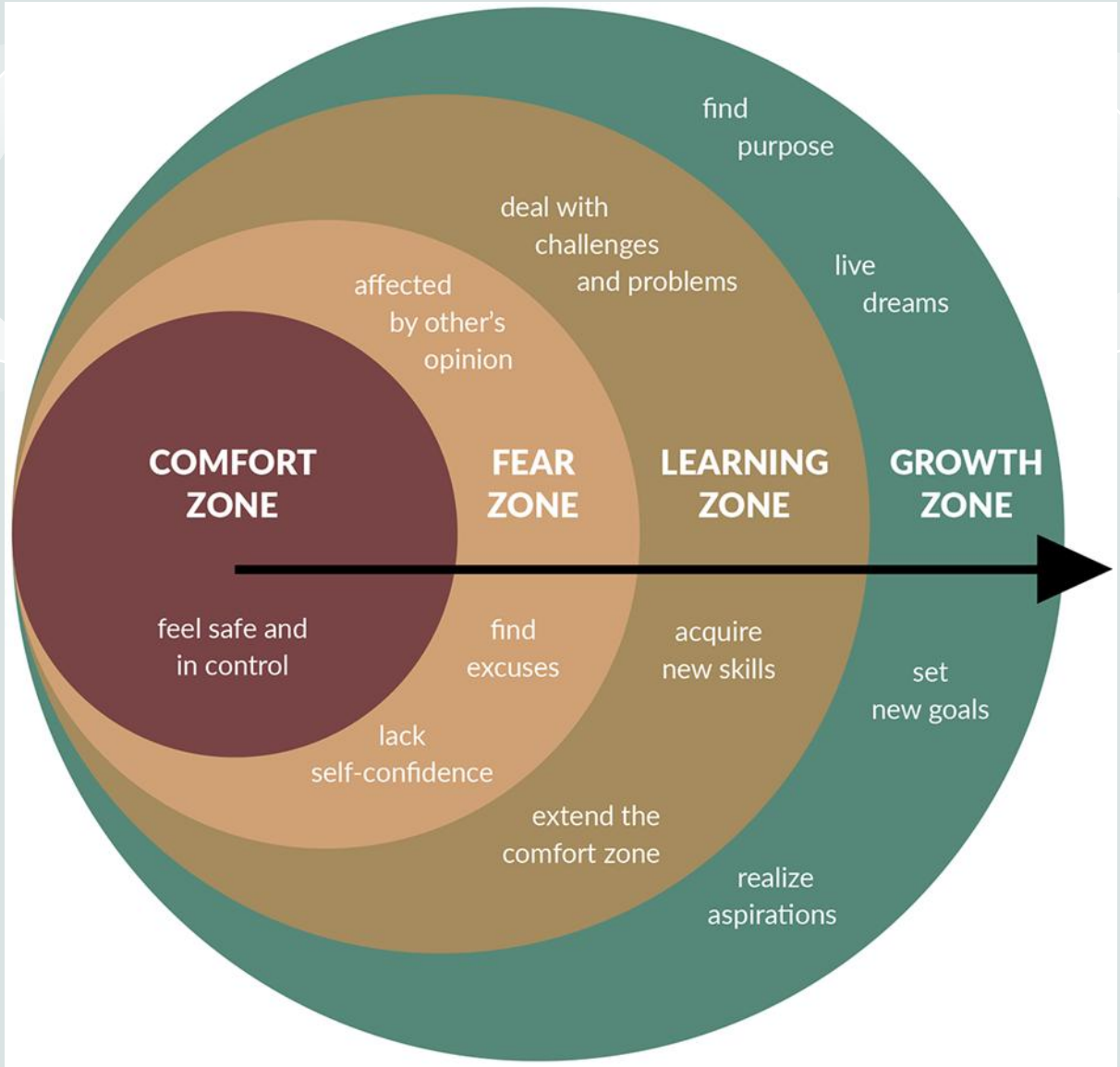
The following statement summarizes the main grasp of this presentation:

“Going beyond the Comfort Zone of the Automatic Adaptive Quadrature: Interlacing of Comfort Zone, Fear Zone, Learning Zone and Growth Zone Knowledge.”



L. Riley, From Comfort to Growth!, Updated: Jun 8, 2023, https://www.museandminds.co.za/post/from-comfort-to-growth-1

Calculus versus Modern Mathematical Analysis

- The connection between Calculus and Modern Mathematical Analysis is foundational:
  - ***Calculus*** provides the ***elementary concepts*** (differentiation/integration) and ***computational methods***.
  - ***Modern Mathematical Analysis*** provides the rigorous logical framework and theoretical proofs that justify why these methods work.
- In contemporary education and practice, these terms often distinguish between application and theory.

Feature	***Calculus*** (*"high level" applications*)	***Modern Mathematical Analysis*** (*"low level" deeper understanding*)
Focus	**How to** calculate results (differentiation/integration)	**Why** the methods work (rigorous proofs)
Methods	Rules, algorithms and computational procedures	Formal definitions, theorems and logic
Audience	Engineers, physicists, and applied scientists	Researchers in pure mathematics

Ubiquity of the Integrals Needing Numerical Solution

The pervasiveness of the integrals asking for numerical solutions can be noticed in three different instances.

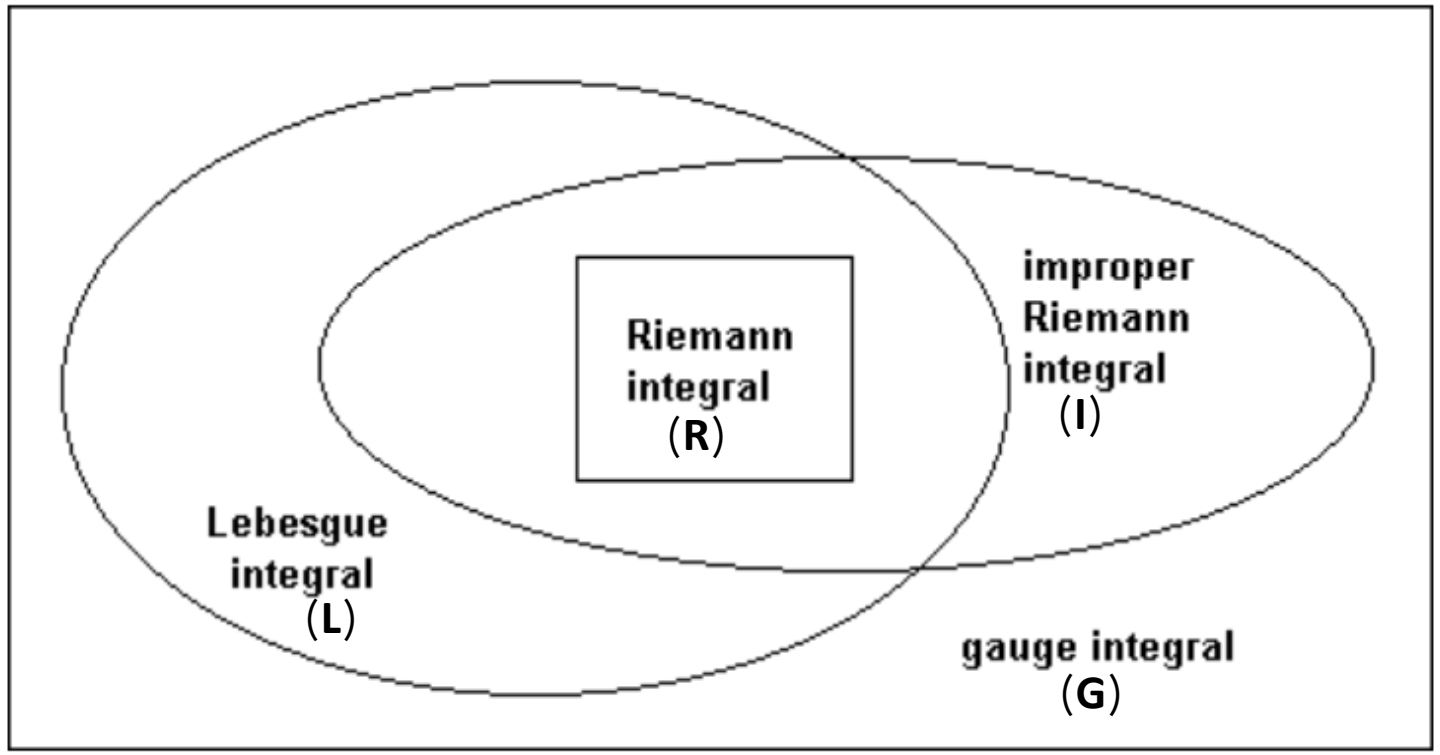
(i) In the realm of the ***classical mathematical physics***, a basic prerequisite of which is the ***problem well-conditioning***, the three classes of solution behaviors (elliptic, parabolic, hyperbolic) are obtained in terms of ***special functions***, each of which involves specific integrals, the overwhelming fraction of which cannot be expressed analytically, hence the ***need of their numerical computation at the abscissas of interest***.

(ii) The myriads of problems arising in the ***present day*** scientific research, high tech engineering, economics, etc., are characterized, as a rule, by various kinds of ***ill-conditionings***, which make imperative the need of the computation of the occurring integrals, under ***harsh data conditioning***.

It is our pleasure to quote the pertinent example of the just ended, outstanding lecture done by our friend, Prof. Hassan Safouhi, concerning subtleties and difficulties to be overcome by the successful computation of Three-Center Nuclear Attraction Integrals, the central topic in the today *ab-initio* molecular orbital calculations.

(iii) Finally, in the problems involving ***numerical modeling***, the occurrence of integrals needing solution **escapes the *a priori* human assessment** of the most reliable paths to the solutions. Here, the ***artificial intelligence*** is to take the lion share of the process of ***supervising the resilience of the computing chain***.

Venn Diagram of Integrable Functions[1]



A Venn diagram for integrals provides a set-like schematic representation of the relationship between types of integrals and coverage of their convergence properties.

$$\mathbf{R} \subset \mathbf{L}, \mathbf{R} \subset \mathbf{I}, \mathbf{I} \cap \mathbf{L} \neq \emptyset, \mathbf{R} \cup \mathbf{L} \cup \mathbf{I} \subset \mathbf{G}$$

$\mathbf{L} \cap \mathbf{I}$ corresponds to absolute convergence

$\mathbf{I} \setminus \mathbf{L}$ corresponds to conditional convergence

G is broader than the union of all previously defined kinds of integrals

[1]Eric Schechter, An Introduction to **The Gauge Integral** also known as the generalized Riemann integral, the Henstock integral, the Kurzweil integral, the Henstock-Kurzweil integral, the HK-integral, the Denjoy-Perron integral, etc. (version of 11 Nov 2009). https://math.vanderbilt.edu/schectex/ccc/gauge/

Putting the Gauge Integral into Proper Perspective (1)

The Venn diagram states that the Gauge integral exhausts the possible set of integrand functions, including all the other kinds of integrals as subsets.

The astonishing fact, which puts the Gauge integral into proper perspective, is its surprising simplicity, a little bit more complicated than the Riemann integral and orders of magnitude simpler than the Lebesgue integral – with its far more prerequisite equipment (sigma-algebras, measures, measurable sets, measurable functions).

To illustrate that, we start with the following definition of the proper Riemann integral[(1)]:

Let $f : [a, b] \to \mathbb{R}$ be some function, and let V be some number. We say that V is the **Riemann integral** of f, written $V = \int_a^b f(t)\,dt$, if for each number $\varepsilon > 0$ there exists a corresponding number $\delta > 0$ with the following property: Whenever n is a positive integer, and $t_0, t_1, t_2, \ldots, t_n$ and $s_1, s_2, \ldots, s_n$ are some numbers satisfying

$$a = t_0 \le s_1 \le t_1 \le s_2 \le t_2 \le \cdots \le t_{n-1} \le s_n \le t_n = b$$

and $\boldsymbol{t_i - t_{i-1} < \delta}$ for all $\boldsymbol{i}$, then $\left| V - \sum_{i=1}^{n} f(s_i)(t_i - t_{i-1}) \right| < \varepsilon.$

[(1)]Eric Schechter, *op. cit.*

Putting the Gauge Integral into Proper Perspective[(1)] (2)

A valid definition of the Gauge integral, which emphasize the similarity with the Riemann integral is[(1)]:

Let $f : [a, b] \to \mathbb{R}$ be some function, and let V be some number. We say that V is the **gauge integral** of f, written $V = \int_a^b f(t)\,dt$, if for each number $\varepsilon > 0$ there exists a corresponding function $\delta : [a, b] \to (0, +\infty)$ with the following property: Whenever n is a positive integer, and $t_0, t_1, t_2, \ldots, t_n$ and $s_1, s_2, \ldots, s_n$ are some numbers satisfying

$$a = t_0 \le s_1 \le t_1 \le s_2 \le t_2 \le \cdots \le t_{n-1} \le s_n \le t_n = b$$

and $\boldsymbol{t_i - t_{i-1} < \delta(s_i)}$ for all $\boldsymbol{i}$ then $\left| V - \sum_{i=1}^{n} f(s_i)(t_i - t_{i-1}) \right| < \varepsilon.$

The single difference: in the Riemann integral $\boldsymbol{\delta}$ is a positive constant, while in the Gauge integral, $\boldsymbol{\delta(s_i)}$ denotes a **gauge** function. The collection of numbers $\boldsymbol{n, s_i, t_i}$ is called a **tagg division** (or a *tagg partition*). The numbers $\boldsymbol{s_i}$ are called the **tags**. The tagg division is called $\boldsymbol{\delta}$**-fine** if it fulfills the condition $\boldsymbol{t_i - t_{i-1} < \delta(s_i)\ \forall\ i}$.

Cousin's Lemma states that *for any gauge* $\boldsymbol{\delta}$**,** there exists *at least one* $\boldsymbol{\delta}$**-fine** tagged division.

[(1)]Eric Schechter, *op. cit.*

The Adaptive Quadrature Is an Appropriate Approach to the Numerical Solution of the Gauge Integrals

- First, the Gauge integral is a tagged partition generalization of both the proper and improper Riemann integrals, for which the adaptive quadrature was previously developed.
- Second, the ***δ*-fine** partition of a particular Gauge integral ***closely follows the specific variation pattern*** of the ***integrand function***: it gets ***sparse tags*** over the ranges of ***slow*** integrand variations and it gets ***dense tags*** over the ranges of ***fast*** integrand variations (e.g., integrand ***singularities***, or ***violent integrand oscillations***).
- Third, ***all*** the known theorems established within the Integration Theory have been proved to ***hold true*** for the Gauge integral. In particular, the ***additivity property*** of the Gauge integral (which provides the foundational basis of the adaptive quadrature) ***holds true***.
- Since the Gauge integral recovers as particular cases ***all*** the previously defined kinds of the one-dimensional integrals, we conclude that the ***adaptive quadrature*** is the ***natural approach*** to the numerical solution of the Gauge integral.
- A reliable AAQ solution yields, within the requested input accuracy specifications, a tagged ***δ*-fine** partition of the integration range of the resolved Gauge integral.

Resolving Paths to Gauge Integral Adaptive Quadrature

- The automatic adaptive quadrature (AAQ) of the the Gauge integrals (GI), aimed at resulting into an ***AAQ method***, is a many stage process asking for the consideration of both ***large scale features*** and ***detailed objectives***.
- Large scale features are, e.g., the mathematical formulation of the GI as a Calculus problem, the parameter set characterizing the resolving algorithm, the computational tools serving to the derivation of the final output, the qualified output assessment.
- In the sequel, we assume that, once the specific steps within the chain resulting in a resolving algorithm have been decided, a ***numerical solution*** using ***double precision floating point computations*** is obtained. Therefore, ***the strong and weak features of the floating point computation are basic factors*** entering the method ***validation***.
- In a nutshell, the ***generic steps*** resulting into an AAQ method involve:
  - Statement of the GI to be solved.
  - Specification of the input data needed for solution:
    - Compulsory input set
    - Optional input set
  - Formulation of the resolving algorithm.
  - Algorithm implementation into a computer code, within a high level programming language
  - Code execution and validation
  - Assessment of the ***strong*** and ***weak*** features of the developed AAQ method.

Numerical Quadrature of the Gauge Integrals: Minimal Input Data Set

Formal statement

- A numerical solution is sought of the one-dimensional Gauge integral (GI),

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

under the implicit assumption that I ***exists*** and is ***finite***. Here:

- $a, b \in \mathbb{R}$ denote the ends of the integration interval;
- $f: [a, b] \to \mathbb{R}$ denotes the ***integrand function***, $f(x)$.

Input to GI

- Is provided ***by the user***. He/she is bounded to provide ***with pinpoint accuracy*** the ***needed input*** to the code.
- The compulsory (***minimal***) input involves three kinds of data:

$$\{\bar{a}, \underline{b}, f, \varepsilon_a, \varepsilon_r\} \qquad (2)$$

- The ***pair*** $\{\bar{a}, \underline{b}\}$ provides the ***floating point specifications*** of the ***integration limits*** a and b, respectively;
- f provides the ***algorithm*** enabling the computation of $f(x)$;
- The values ε_a and ε_r denote the maximum admissible ***absolute***, respectively ***relative***, errors of the computed output to I.

Two Basic Quantities

- Over a ***finite*** integration interval $[\bar{a}, \underline{b}]$, the numerical solution of the GI (1) involves two quantities: the ***centre*** (c) and the ***half-width*** (h) of $[\bar{a}, \underline{b}]$:

$$c = \frac{(\underline{b}+\bar{a})}{2}, \quad h = \frac{(\underline{b}-\bar{a})}{2} \qquad (3)$$

Three Great Precursors: 1. QUADPACK

- The **QUADPACK**[(2)] package provides, for half a century, the ***state-of-the-art software*** for the ***automatic adaptive quadrature*** (AAQ) solution of the Riemann integrals.
- It implements two classes of numerical procedures: (a) a set of ***master procedures*** (subroutines), driving the flow of the AAQ process and (b) specialized ***slave procedures*** (fully characterized quadrature sums), asked by corresponding master procedures.
- Notice is to be made of two contradictory features of the QUADPACK package:
  - (i) It provides a wealth of ***perennial reference ideas*** serving as solid starting points for further developments of the AAQ methods.
  - (ii) The ***heavy use of rules of thumb*** induces the ***fragility*** of many of the QUADPACK AAQ decisions, due to their ***critical dependence on the user's expertise*** in the choice of the right resolving master procedure from the package at hand.
- In this respect, ***our proposal*** is to use ***input validation procedures***, at suitable places of the control decision tree. This addition enforces highly reliable ***Bayesian inferences*** on the choice of the appropriate AAQ ***resolving path***.

[(2)]R. Piessens, E. de Doncker-Kapenga, C.W. Ueberhuber, and D.K. Kahaner, QUADPACK: A Subroutine Package for Automatic Integration (Springer Series in Comp. Math., vol. 1, Springer Verlag, Berlin, 1983).

Three Great Precursors: 2. DE Transform

- The ***Double Exponential* (DE) *Transform***[3] provided an empirical proposal that resulted in ***significant increase*** of the ***efficiency and coverage*** of the ***exponentially converging trapezoidal rule***.

  To our knowledge, there are three noticeable facts about the DE Transform:

(i) The DE was bluntly refused for consideration by the QUADPACK team (cf. Mori[4]).

(ii) Research done in the Trefethen's group[13] significantly clarified and improved the efficiency of the DE Transform.

(iii) ***Experimental mathematics high precision investigations***[5]-[7] assessed the DE Transform as the ***best*** existing approach to the solution of ***difficult integrals***.

[3]H. TAKAHASI and M. MORI, Double Exponential Formulas for Numerical Integration, PM. RIMS, Kyoto Univ. **9** (1974), 721-741

[4]M. Mori, Discovery of the Double Exponential Transformation and its Development, Publications of RIMS, Kyoto University, **41**(2005) 897–935.

[5]D. H. Bailey, K. Jeyabalan, and X. S. Li, *A comparison of three high-precision quadrature schemes*, Experiment. Math., **14** (2005), 317–329.

[6]D. H. Bailey, High-Precision Numerical Integration and Experimental Mathematics, https://interval.louisiana.edu/conferences/2007_Stenger/Slides_of_talks/dhb-integrals.pdf

[7]D. H. Bailey, High-Precision Software Directory, Updated: 5 October 2025, https://www.davidhbailey.com/dhbsoftware/

Three Great Precursors: 3. Chebfun

- **The Chebfun project** (see[8] for a printed version, or the 2017–2023 online documentation updates[9]), developed since 2002 at Oxford University under the leadership of L.N. Trefethen, has become a broad multidisciplinary open source project. Its basic idea has been formulated by L.N. Trefethen as follows[10]: "Floating point arithmetic has been a triumphant success for computing with real numbers. The idea behind Chebfun is to do something analog for computing with functions."
- To this aim, the Chebfun software was implemented in the frame of the Matlab programming language by overloading the Matlab double precision discrete operations for vectors and matrices to analogous continuous operations for functions and operators. A wealth of unparalleled results have been reported so far (see, e.g., Refs.[11]-[13]). We feel that Chebfun implements a ***smart big data approach*** to the solution of adaptive quadrature.
- Unfortunately, there are sensitive aspects of Matlab's use: the expensive Matlab proprietary license and limitations induced by political sanctions.

[8]T.A. Driscoll, N. Hale, L.N. Trefethen, Chebfun Guide, 1st Ed., For Chebfun version 5, 212pp. (2015) https://www.chebfun.org/docs/guide/chebfun_guide.pdf
[9]Documentation. Chebfun Guide, https://www.chebfun.org/docs/guide/
[10]L.N. Trefethen, Chebfun as a software project, https://people.maths.ox.ac.uk/trefethen/chebfun_icms14.pdf
[11]L.N. Trefethen, Is Gauss Quadrature Better than Clenshaw-Curtis? SIAM Review 50(1), 67–87 (2008), https://doi.org/10.1137/060659831.
[12]N. Hale, L.N. Trefethen, Chebfun and numerical quadrature, Sci. China Math., 55(9) (2012) 1749–1760, https://www.doi.org/10.1007/s11425-012-4474-z
[13]L.N. Trefethen and J.A.C. Weideman, The Exponentially Convergent Trapezoidal Rule, SIAM Review, vol. 56, no. 3, 385–458 (2014). https://doi.org/10.1137/130932132

Lessons Learned from the Three Precursors: 1. QUADPACK

1. A valuable basic assumption made **within the QUADPACK package** is that the *a priori* knowledge of the integral to be solved is ***essential*** for the derivation of a reliable output.

   Nevertheless, the ***frozen*** implementation of this knowledge, in a menu *à la carte*, asks for the ***expert knowledge by the user***, of ***both*** the problem to be solved ***and*** the existing subroutine software menu. ***Low level expertise*** or ***accidental lack of attention*** may result in ***harsh code failure***.

   Moreover, the occurrence of ***very few*** (if any) ***points of discontinuity*** of the integrand function $f(x)$ and/or its derivatives is assumed.

   Under the occurrence of ***cancellation by subtraction*** (CANSUB), the QUADPACK EoC global criterion cannot guarantee the ***stop*** of the computation process at the ***minimum*** of the sum of the truncation and of the round-off errors. As a rule, this case ends with a useless diagnostic of ***catastrophic precision loss*** of the floating point computations.

Lessons Learned from the Three Precursors: 2. DE Transform

2. The **Double Exponential (DE) Transform** illustrates the paradox that the ***performances of the simplest possible algorithm*** (the iterated trapezoidal rule) may be at the level of the ***most sophisticated ones*** (Gauss, Clenshaw-Curtis). Of course, this is only possible for ***analytic integrand functions*** characterized either by monotonic or slowly oscillatory variation over the integration domain.

   Yet, there is a very important lesson learnt from the consideration of the DE transform. Under the occurrence of ***general*** integrands over integration intervals extending at infinity in one or both directions, the build up of a trapezoidal like partition toward the corresponding point at infinity is essential for the ***cheap definition*** of a convenient ***cut-off*** of the infinite integration end, while yielding ***reusable*** information within the AAQ algorithm.

Lessons Learned from the Three Precursors: 3. Chebfun

- Within the **Chebfun project**, the preferred Matlab driven implementation of the numerical computation of integrals (1) assumes the ***Clenshaw-Curtis quadrature*** over the ***standard*** integration interval $[-1,1]$. Then the $(n+1)$-knot polynomial or piecewise polynomial interpolation of the integrand function $f(x)$ is done at the set of Chebyshev points: $\{s_j = \cos(n^{-1}j\pi)\,|j = 0,1,\cdots,n\}$, enabling the use of Fast Fourier transform (FFT) that asks for $\mathcal{O}(n\log n)$ operations only (with a small multiplicative constant).

  The possibility to raise n up to degrees of millions, while asking for small computing time, enables the derivation of numerical solutions for exceptionally complicated behaviors of the integrand functions $f(x)$.

  Efficient Gauss quadrature capabilities (Gauss-Legendre, Gauss-Chebyshev, Gauss-Jacobi, Gauss-Hermite, Gauss-Laguerre) have been implemented in Chebfun over corresponding ***default*** integration domains.

  Similar to the QUADPACK package, the mapping $[a,b] \to [-1,1]$ involves the floating point computation of values for the center c and the half-width h, Eq. (3), of $[a,b]$.

  Catastrophic cancellation by subtraction, hence the derivation of ***useless output*** for the actual problem of interest occurs iff $|b-a| \ll \max\{|a|,|b|\}$.

Educated Guesses and *a priori* Knowledge – Pillars of Quadrature Code Resilience

- The development of the concept of the ***Gauge integral*** (GI) is the last instance in the three century long chain of ***educated guesses*** that resulted in the present day Calculus and Modern Mathematical Analysis.

  The AAQ resolving chain of the Gauge integrals enables ***explicit definition*** of the gauge function $\delta(x)$.

- The today three classes of ***quadrature algorithms*** (using constant step, Gauss like, or Clenshaw-Curtis like quadrature sums) are consequences of educated guesses, built upon previously developed knowledge.
- Under ***the lack*** of an *a priori* ***knowledge*** of the detailed properties of the graph of the integrand function $f(x)$, the derivation of a ***numerical solution*** of the GI (1) is possible under the provision of the ***minimal input*** (2). Of course, a resolving ***resilient code*** will have to go through the ***longest possible chain of decisions*** enabling the right path to the solution.
- The *a priori* knowledge of the points of ***irregular behaviour*** in the graph of $f(x)$ may secure ***two levels of code acceleration***:

  •• the ***bare specification*** of the ***location of the offending abscissas***: enables the ***direct*** (***fastest***) build up of the ***roots*** of the ***forest of decision trees*** controlling the resolving process;

  •• the provision of the ***quantitative parameters*** characterizing the ***irregular integrand behaviours***: enables the definition and use of ***integrand adapted*** quadrature knots for the ***appropriate Gauss-like integrands*** (like, e.g., in the Chebfun library) that are characterized by ***resolving algorithms showing the maximum possible efficiency.***

Sensitive Floating Point Computations in Automatic Quadrature (1)

- The numerical evidence reported by the authors of the QUADPACK, DE Transform and Chebfun quadrature points to output accuracies of the implemented numerical codes up or near to the ***machine accuracy***.

  The general feeling is that the ***precision loss*** generated by the floating point computations could hardly be expected to be of significant importance.

  In fact, the reliability and portability of the floating point computations proved to be of fundamental importance both for the hardware and software providers, to be formalized in an international standard. The IEEE 754 standard, originally established in 1985 and refined in 2008 and 2019, respectively, was followed by a number of deep investigations addressing the computing with floating point numbers (see, e.g., [14],[15],[16]).

  Going along these lines, we have identified several Achilles' heels in the existing implementations, which are briefly addressed below.

- (1) Within the ***quadrature sums of constant step*** (midpoint, trapezoidal, Simpson) the output asks for the ***computation of the half width*** h, Eq. (2).

  (2) Within the Gauss type and Clenshaw-Curtis type quadrature sums over finite ranges, the current input interval $[\overline{a}, \underline{b}]$ is mapped onto the standard integration interval $[-1, 1]$ by means of the transformation of ***independent variable***, $x = c + h\xi,\ x \in [\overline{a}, \underline{b}], \xi \in [-1,1]$, where the quantities c and h are given by (2).

  If the integration ends $\overline{a}$ and $\underline{b}$ fulfil the condition $|\underline{b} - \overline{a}| \ll \max\{|\overline{a}|, |\underline{b}|\}$, then ***the single step*** addressing the computation of h induces ***catastrophic cancellation by subtraction***, which results in ***doubtful*** computed output!

  The remedy to this difficulty: is to use ***quadruple precision*** for ***each*** of the input values $\overline{a}$ and $\underline{b}$.

[14]IEEE Computer Society (2019-07-22). IEEE Standard for Floating-Point Arithmetic. IEEE STD 754-2019. IEEE. pp. 1–82. https://doi.org/10.1109/IEEESTD.2019.8766229

[15]D. Goldberg (March 1991). "What Every Computer Scientist Should Know About Floating-Point Arithmetic". Edited, 94 page, document. https://web.archive.org/web/20171011072644/http://www.cse.msu.edu/~cse320/Documents/FloatingPoint.pdf

[16]V. Lafage, Revisiting "What Every Computer Scientist Should Know About Floating-point Arithmetic", 13 pp., 4 Dec. 2020, https://doi.org/10.48550/arXiv.2012.02492

Sensitive Floating Point Computations in Automatic Quadrature (2)

- (3) The QUADPACK global end of computation (EoC) criterion is ***fragile*** [17].

  Indeed, under the occurrence of ***oscillatory*** integrand variation involving both ***positive and negative*** computed integrand values under the area of the graph of $f(x)$ over $[\overline{a}, \underline{b}]$, ***partial*** cancellation by subtraction (CANSUB) occurs in the computed global quadrature sum. Then the global EoC criterion may ***fail*** to stop the computations at the level of discretization at which the ***decreasing*** global truncation error ***equates*** the ***increasing*** global round off error. Under further discretization refinement, the latter ***dominates*** the behaviour of the global AAQ error, which grows indefinitely at the expense of the round off error component , such that ***fatal loss of precision*** is diagnosed under ***useless output***.

  The solution to this problem, which often occurs under ***highly*** oscillatory integrands $f(x)$, is to ***add*** the supplementary task of computing over $[\overline{a}, \underline{b}]$ the integral of $|f(x)|$. Since the set of values of the modulus $|f(x)|$ is ***free*** of CANSUB effects, the use of a global EoC criterion, formulated in terms of this quantity is ***safe*** and results in ***reliable*** output.

- (4) In QUADPACK, the activations of ***convergence acceleration procedures*** are decided by the use of ***rules of thumb***, which are open to failure.

  Within the present AAQ method, the definition of the ***extension*** of the ***basin of attraction*** of a ***resolved endpoint integrand singularity*** follows from the condition of ***monotonic increase***, away from the singular point, of the local values of the gauge function $\delta(x)$. The place at which this increasing process ***stops*** provides an ***accurate*** quantitative measure of the second end of the integration range starting at the endpoint singularity, over which the convergence acceleration procedure is to be activated.

[17]Gh. Adam, S. Adam, Prerequisites for Artificial Intelligence Driven Automatic Adaptive Quadrature. *Phys. Part. Nuclei* **56**, 1255–1263 (2025). https://doi.org/10.1134/S1063779625700339

Subrange Decision Tree Frame for AI AAQ

DT Frame

- The iterative AI AAQ up-down path to the derivation of a numerical solution of the RI (1) is driven by the implementation of a *specific* ***decision tree*** (DT).

SSDT

- Under the provision of the *minimal input in floating point computation*

$$\{\overline{a}, \underline{b}, f(x), \varepsilon_a, \varepsilon_r\}, \qquad (17)$$

the AI driven AAQ rests on the build up of a single DT, the elements of which are (sub)ranges of $[\overline{a}, \underline{b}]$ – whence the acronym SSDT, ***single subrange decision tree***.

This SSDT should be able to be derived from the scratch. Alternatively, under the provision by the user of input concerning the *conditioning* of $f(x)$ at the endpoints $\overline{a}$ and $\underline{b}$, adequate ***input validation*** procedures are used.

FSDTs

- If $f(x)$ ill-conditioning was resolved at one or more inner isolated abscissas inside $(\overline{a}, \underline{b})$ during the AAQ solution implementation, then the AI AAQ solution builds up dynamically a ***forest of subrange DTs*** (FSDTs).

Alternatively, if an *a priori* study conducted by the user evidenced $f(x)$ ill-conditioning at one or more inner isolated abscissas, then the AI AAQ solution ***is started with a FSDTs***, subject to specific input validation.

Input Validation

- Under every of the alternatives described above, the ***input validation*** procedures provide objective assessment of the decision tree structure entries. Hence the input to the AI AAQ is ***robust***.

Robust Status Assessments of SSDT Root Ends (1)

Task

- Define ***from scratch*** $\left\{\tau, f(\tau), \varphi_\tau | \tau \in \{\overline{a}, \underline{b}\}\right\}$ for the SSDT root $[\overline{a}, \underline{b}]$.
- ***Values*** $\{\tau, f_0 = f(\tau)\}$ are straightforward.
- The derivation of $\{\varphi_\tau\}$ need elaborate procedures, over lateral local proximity neighborhoods of the reference abscissa τ, inside $[\overline{a}, \underline{b}]$, which are discussed below.

Meaningful $\{\varphi_\tau\}$ diagnostics

- The occurrence of two fundamentally different values of f_0 define **specific approaches** to the derivation of $\{\varphi_\tau\}$ diagnostics:
- (i) **Root end of the kind 1**, iff $|f_0| = +\infty$ **.** Its assessment involves computed $f(x)$ values within an ***open*** lateral neighbourhood of τ. Yields BL1 diagnostic (label -1).
- (ii) **Root end of the kind 2**, iff $|f_0| < +\infty$ **.** This adds the pair $\{\tau, f_0\}$ to the open lateral neighbourhood discretization defined in the case (i), resulting in a ***closed*** lateral neighbourhood of τ.

  The scrutiny of the variation of $f(x)$ inside this set results into two possible root end status (RES) diagnostics:

  (ii1) A milder ***nonlinear*** integrand variation around τ. Yields BL2 diagnostic (label -2).

  (ii2) A ***smooth*** RES around τ (label 2).
- **Root end of the kind 3:** an ***infinite end*** a or b associates a label 3 diagnostic.

Robust Status Assessments of SSDT Root Ends (2)

"Magic" open inner local discretizations near τ

Generic abscissas

- Are suggested by the existing evidence on the philosophy of the Gauge integral concerning the δ-fine setting of integrals with endpoint singularities:

$$X_P = \{x_{2^p} = \tau + 2^p \sigma \rho \mid p = 0,1, \dots, P\}$$

- Here, P denotes an as yet undefined upper bound of the discretization.
- $\sigma = +1$ iff $\tau = \overline{a}$ and $\sigma = -1$ iff $\tau = \underline{b}$ point to ***increasing***, respectively ***decreasing*** x_{2^p} values inside X_P.

Machine numbers subtlety

- The parameter ρ denotes a convenient approximation of the elementary distance between two neighbouring (almost everywhere) machine number abscissas:

$$\rho = \max\{\delta_0, |\tau|\}\, \varepsilon_0, \qquad \delta_0 = 2^{-9}\, \varepsilon_0$$

The parameter ε_0 denotes the ***machine epsilon***, assumed here equate the value defined by the modern Fortran standards for double precision computations.

Robust Status Assessments of SSDT Root Ends (3)

Characteristic sets defined over X_P

Integrand values

- The computation of the integrand function values over the set X_P yields the set:

$$F_P = \{f_{2^p} = f(x_{2^p}) \mid p = 0,1, \dots, P\}.$$

- Each newly computed value f_{2^p} is checked for ***finiteness***, $|f_{2^p}| < +\infty$.
- If this condition is infringed, then the x_{2^p} abscissa defines an inner point that contributes to the ***inception*** or ***extension*** of a dynamically built ***forest of subrange decision trees*** (FSDTs). The assessment of the status of the pair of roots ending at x_{2^p} is started as a new input validation process.

First order differences

- Given the validated pair set $\{X_P, F_P\}$, we get the set of ***first order differences***:

$$S_P = \left\{s_{2^{p-1},2^p} = 2^{-p+1}\sigma(f_{2^p} - f_{2^{p-1}}) \mid p = 1,2, \dots, P\right\}.$$

These quantities provide (up to a constant factor ρ^{-1}), the ***local integrand slopes*** over the set X_P .

Second order differences

- Given the validated pair set $\{X_P, S_P\}$, we get the set of ***second order differences***:

$$C_P = \left\{c_{2^{p-2},2^{p-1},2^p} = 2^{-2p+3}(f_{2^p} - 3f_{2^{p-1}} + 2f_{2^{p-2}}) \mid p = 2,3, \dots, P\right\}.$$

These quantities provide (up to a constant factor $(3\rho^2)^{-1}$), the ***local integrand curvatures*** over the set X_P .

Robust Status Assessments of SSDT Root Ends (4)

Setting the status of a **root end of the kind 1**

Basic hypothesis

- The singularity of $f(\tau)$ is the ***unique source*** of integrand ill-conditioning at τ.
  Then the quadrature sums ***slowly converge*** over ranges ending at or near τ.
  This can be cured with the help of a ***convergence acceleration algorithm***.

Assessment procedure

- A two step forward predictor–corrector procedure is used. It checks the fulfillment of the ***strict monotonicity*** of the sets F_P, S_P, C_P at the minimum possible $P = 3$ value first (predictor) and then at the next $P = 4$ value (corrector).

Conclusion

- It follows that the assessment of a BL1 diagnostic $\varphi_\tau = -1$, over a "magic" minimum inner local neighbourhood discretization asks for the computation of an extra set of ***five integrand values*** $\{f_1, f_2, f_4, f_8, f_{16}\}$ $(P = 4)$.
- The validity of such an inference over the missing integrand values in the five value set follows from the continuity properties of the integrand function under the fulfillment of the strict monotonicity properties.

Robust Status Assessments of SSDT Root Ends (5)

Setting the status of a **root end of the kind 2**

Outcome of enhanced input

- The availability of a ***close proximity*** neighbourhood of τ for analysis secures the extension of the open "magic" sets X_P, F_P to their lateral closures

$$\widetilde{X_P} = \{\tau \cup X_P\}, \quad \widetilde{F_P} = \{f_0 \cup F_P\}\,.$$

- The ***finiteness*** of ***all*** the quantities entering $\widetilde{X_P}$ and $\widetilde{F_P}$ is compatible with ***two kinds*** of ***local integrand*** behaviour near τ, which enable effective quadrature rule solutions:
  - •• local ***linear*** integrand behaviour (LLIB),
  - •• local ***nonlinear*** integrand behaviour (LNIB).

Opposite length scales over the machine number set

- The reliability of the AI LLIB diagnostic is enhanced provided the analysis is done over ***as large as possible*** length scale machine number ranges around τ.
- The reliability of the AI LNIB diagnostic is enhanced provided the analysis is done over ***as small as possible*** length scale machine number ranges around τ.
- These two features ***give prevalence*** to the study of the ***LLIB case first***.

Robust Status Assessments of SSDT Root Ends (6)

Linear least squares solution of **LLIB alternative**

Pillars of the LLIB diagnostic

- The analysis of a general set of $m+1 \ \ (m \geq 3)$ input data (x_i, f_i) goes through three basic steps:
  - (A) Definition of the three lowest degree monic orthogonal polynomials by Gram-Schmidt orthogonalization.
  - (B) Derivation of the best fitting coefficients of the linear combination of orthogonal polynomials from the minimization of the least squares (LSQ) fitting functional.
  - (C) Check if the curvature of the fitting functional is negligible.

Minimal sampling

- The minimum sampling set from within $\{\widetilde{X_P}, \widetilde{F_P}\}$ involves the four pairs

$$\{(\tau, f_0) \cup \{(x_{2^p}, f_{2^p}) | \ p = q-2, q-1, q | 0 \ll q\}\} .$$

LSQ solution

- The LSQ solution finds that the curvature of this distribution is proportional to

$$2^{-2q}(7f_0 - 4f_{2^{q-2}} - 8f_{2^{q-1}} + 5f_{2^q}), \forall q \geq 2 .$$

- Therefore, the condition for the existence of a local linear integrand behaviour near τ is the ***negligibility*** of this quantity. Thus, a LLIB diagnostic asks for the computation of ***three*** integrand values at abscissas of labels $\{2^p | \ p = q-2, q-1, q\}$.

Robust Status Assessments of SSDT Root Ends (7)

LNIB diagnostic BL2 (Boundary layer of kind 2)

Approach

- This problem arises only provided the LLIB setting resulted in a negative answer.
- The assessment of a BL2 diagnostic is attempted over BL1-like primary data sets F_P, S_P, C_P, within a ***backward*** predictor–corrector procedure.

Assessment procedure

- The AI idea is to reuse the already available data generated within the tentative solution $\varphi_\tau = 2$ (smooth case) at the label set $\{2^p \mid p = q-2, q-1, q\}$, as input to the backward predictor step under the reduction to a minimum of the remaining set at the lowest label $\{0, 1, \ldots, q-3\}$ set of data. The compromise value $q = 5$ reaches this goal by setting the backward predictor step at labels $\{2, 3, 4, 5\}$, and the backward corrector step at labels $\{0, 1\}$ inside the sets F_P, S_P, C_P.
- The backward corrector step successfully ends with the $\varphi_\tau = -2$ diagnostic provided it is confirmed for the closure of F_P, S_P, C_P with the endpoint values f_0, $s_{0,1}$ and $c_{0,1,2}$, respectively.

Conclusion

- It follows that the assessment of a BL2 diagnostic $\varphi_\tau = -2$ at τ asks for the computation of an extra set of ***six integrand values*** $\{f_1, f_2, f_4, f_8, f_{16}, f_{32}\}$ $(P = 5)$.

Assessment of the basin of the endpoint singularity dominance

Basin extension

- The dominance of the boundary singularity over the other integrand properties occurs over a ***macroscopic distance*** away from τ. A convergence acceleration algorithm is useful precisely over this singularity dominance range. The adequate assessment of its extension is of the utmost importance.

Assess-ment criterion

- The basin of the endpoint singularity dominance away from τ is defined by the maximal P value at which the ***strict monotonicity*** is observed at every available $p \leq P$ value within each of the sets F_P, S_P, C_P.

Maximal range

- This procedure sets the ***maximal range*** $[\tau, \tau + 2^P \sigma\rho]$ over which the ***convergence acceleration procedure*** is to be ***started*** and ***refined*** by ***bisection*** until the enhanced accuracy following from extrapolation reaches the Global End of Computation criterion.

Procedure efficiency

- The storage of the computed abscissas and integrand values defined during the assessment of the maximal range secures the ***minimal number of integrand evaluations*** over this range.
- Assessment of the ***increasing monotonic behaviour of the Gauge function*** $\delta(x)$ ***away from the singular end*** provides the ***final validation criterion*** for the definition of the extension of the integrand singularity dominance.

AI Root-End-Settings Generate an Articulated Initial AAQ Stage

- The **16 *possible root end instantiations resolved by AI analysis*** may be grouped into ***four distinct classes of root end pairs***, each being characterized by a ***distinct initial resolving path***.
  - Class **Smooth – Smooth**: $\{(2,2),(2,3),(3,2),(3,3)\}$. **Single root** $[\overline{a},\underline{b}]$, compatible with the use of a ***single closed Symmetric Interpolatory Quadrature Sum*** **(SIQS)**.
  - Class **BL* – Smooth**: $\{(-1,2),(-1,3),(-2,2),(-2,3)\}$. **Forest**, comprising **two adjacent tree roots**: $(\overline{a},X_{PR}]\cup[X_{PR},\underline{b}]$, where X_{PR} denotes the **right limit** of the basin of the endpoint singularity dominance starting at $\overline{a}$. The root $(\overline{a},X_{PR}]$ asks for ***an open SIQS at*** $\overline{a}$ ***, able to secure convergence acceleration. The root*** $[X_{PR},\underline{b}]$ ***is compatible with the use of a closed SIQS.***
  - Class **Smooth – BL***: $\{(2,-1),(2,-2),(3,-1),(3,-2)\}$. Is the **symmetric** of the previous one. Hence, **forest** comprising **two adjacent tree roots,** $[\overline{a},X_{PL}]\cup[X_{PL},\underline{b})$, etc.
  - Class **BL* – BL***: $\{(-1,-1),(-1,-2),(-2,-1),(-2,-2)\}$. **Forest**, comprising, in general, **three adjacent tree roots**: $(\overline{a},X_{PR}]\cup[X_{PR},X_{PL}]\cup[X_{PL},\underline{b})$. The roots ending at $\overline{a}$ and $\underline{b}$, respectively, use half open SIQSs able to secure convergence acceleration. The **inner** root, $[X_{PR},X_{PL}]$, is compatible with the use of a **closed** SIQS. In the **exceptional case** $[X_{PR}=X_{PL}]$, this **root is absent**.

This articulated structure recovers the previously conceived basic master procedures, while eliminating completely the danger of artefacts generated by the use of rules of thumb.

An AI Related Open Question

- Fundamental inferences from this investigation:
  - **There is a unique path to the derivation of a resilient solution to the automatic adaptive quadrature of a Gauge Integral through AI decisions, which depends on the *a priori* knowledge of the problem to solve.**
  - We are reluctant that AI LLM implementations would be appropriate to this aim.

Thank you for your attention !

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