

GAUSS'S GAUSSIAN QUADRATURE

J. M. Sanz-Serna

Universidad Carlos III de Madrid

METHODVS NOVA
INTEGRALIVM VALORES PER AP-
PROXIMATIONEM INVENIENDI.

AUCTORE

CAROLO FRIDERICO GAUSS

SOCIETATI REGIAE SCIENTIARVM EXHIBITA D. 16. SEPT. 1814.

In this presentation, parts in black or blue, are taken from Gauss, always keeping his notation. Parts in red are my own comments/explanations.

The memoir, published in MDCCCXV, contains 40 pages and 23 articles.

§1 to §6 (pages 3–11) review carefully the formulas by Cotes (1682–1716) (uniformly spaced nodes).

§7 to §12 (pages 11-21): construction of quadrature formulas
with nonuniformly spaced nodes

- *Determinare $\int y dx$ inter limites datos* when several values of y are known. [No notation for functional dependence like modern $f(x)$.]
- *Integrale sumendum esse ab $x = g$ usque ad $x = g + \Delta$.*
- *$t = \frac{x-g}{\Delta}$, $\Delta \int y dt$, ab $t = 0$ usque ad $t = 1$.*
- *$n + 1$ valores dati $A, A', A'', A''', \dots, A^{(n)}$.*
- *Corresponding values of t : $a, a', a'', a''', \dots, a^{(n)}$.*

- Y functionem algebraicam ordinis n :

$$\begin{aligned}
 & A \frac{(t - a')(t - a'')(t - a''') \cdots (t - a^{(n)})}{(a - a')(a - a'')(a - a''') \cdots (a - a^{(n)})} \\
 & + A' \frac{(t - a)(t - a'')(t - a''') \cdots (t - a^{(n)})}{(a' - a)(a' - a'')(a' - a''') \cdots (a' - a^{(n)})} \\
 & + \text{etc.}
 \end{aligned}$$

such that if t is put equal to a, a', \dots , Y takes the values A, A', \dots [Lagrange interpolating polynomial.]

[To compute $\int Y dt$ begin by rewriting numerators and denominators of fractions in the expression of Y .]

- Introduce

$$\begin{aligned}
 T &= (t - a)(t - a'')(t - a''') \cdots (t - a^{(n)}) \\
 &= t^{n+1} + \alpha t^n + \alpha' t^{n-1} + \alpha'' t^{n-2} + \text{etc.} + \alpha^{(n)}.
 \end{aligned}$$

- then, the *numerators* are $\frac{T}{t-a}, \frac{T}{t-a'}, \dots$ and the *denominators* M, M', \dots the values of $\frac{T}{t-a}, \frac{T}{t-a'}, \dots$ at a, a', \dots [Recall: no notation for functional dependence.] Thus:

$$Y = \frac{AT}{M(t-a)} + \frac{A'T}{M'(t-a')} + \text{etc}$$

[Now we have to (i) find M, \dots and (ii) $\int T/(t-a)dt, \dots$]

- Gauss first computes M in terms of the coefficients α, α', \dots of T and the abscissae a, a', \dots (similar for M' , etc.)]

$$T = t^{n+1} - a^{n+1} + \alpha(t^n - a^n) + \alpha'(t^{n-1} - a^{n-1}) + \text{etc.}$$

$$\begin{aligned} \frac{T}{t-a} &= t^n + at^{n-1} + aat^{n-2} + \text{etc.} + a^n \\ &\quad + \alpha t^{n-1} + \alpha at^{n-2} + \text{etc.} + \alpha a^{n-1} \\ &\quad + \alpha' t^{n-2} + \text{etc.} + \alpha' a^{n-2} \\ &\quad + \text{etc.etc.} \\ &\quad + \alpha^{(n-1)} \end{aligned}$$

In $t = a$, this takes value $na^n + (n-1)\alpha a^{n-1} + \text{etc.} + \alpha^{(n-1)}$.

Thus M equals the value of $\frac{dT}{dt}$ at $t = a$, *uti etiam aliunde constat*.

- Now find *valorem integralis* $\int \frac{T dt}{t-a}$ [using the complicated expression just found for the integrand]:

$$\begin{aligned}
 & \frac{1}{n+1} + \frac{a}{n} + \frac{aa}{n-1} + \text{etc.} + a^n \\
 & \quad + \frac{\alpha}{n} + \frac{\alpha a}{n-1} + \text{etc.} + \alpha a^{n-1} \\
 & \quad \quad + \frac{\alpha'}{n-1} + \text{etc.} + \alpha' a^{n-2} \\
 & \quad \quad \quad + \text{etc.etc.} \\
 & \quad \quad \quad + \alpha^{(n-1)}.
 \end{aligned}$$

[Which does not look too pretty?]

- *Quos terminos ordine sequente disponemus:* [Sum by columns from left to right]

$$a^n + \alpha a^{n-1} + \alpha' a^{n-2} + \text{etc.} + \alpha^{(n-1)}$$

+etc.

$$\frac{1}{n}(a + \alpha)$$

$$\frac{1}{(n + 1)},$$

and it is manifest that this is the result of multiplying T by $t^{-1} + \frac{1}{2}t^{-2} + \frac{1}{3}t^{-3} + \frac{1}{4}t^{-4} + \text{etc.}$, discarding the terms with negative powers of t and replacing t by a . !!!

- Set

$$T(t^{-1} + \frac{1}{2}t^{-2} + \frac{1}{3}t^{-3} + \frac{1}{4}t^{-4} + \text{etc.}) = T' + T'',$$

where T' represents the [n -th degree] polynomial [in t] that the product contains. [Remember this formula. T' and T'' are crucial later. Note their coefficients are linear in the coefficients α, α', \dots , of T . Also recall primes do not mean derivatives.]

- Then $\int \frac{T dt}{t-a}$ equals the value of T' at $t = a$.

- To sum up: if R, R', \dots denote the values of $\frac{T'}{\frac{dT}{dt}}$ at a, a', \dots , [quadrature weights] then $\int Y dt$ is

$$RA + R'A' + R''A'' + R'''A''' + \text{etc.} + R^{(n)}A^{(n)},$$

which multiplied by Δ will be the approximate value of $\int y dx$.

- Theory replicated, now using the variable $u = 2t - 1$ (with values between -1 and $+1$) instead of t (values from 0 to $+1$). Function $U = (u - b)(u - b') \dots (u - b^{(n)})$ replaces T .

- As an example, Gauss finds the weights of Newton-Cotes formulas found with both t and u . The latter exploits symmetry $u \mapsto -u$.
- Next Gauss shows how to express the value of a rational function $\frac{Z}{\zeta}$ at the roots of a polynomial equation $\zeta' = 0$ as a polynomial in those roots. [Recall that the set (field) of rational expressions $\mathbb{Q}(\xi)$ coincides with the set of polynomials $\mathbb{Q}[\xi]$ when ξ is algebraic.] A fully detailed numerical example is given.

§13 to §14 (pages 22-24): error analysis

- For function t^m the error in the integral (from 0 to 1) is $k^{(m)}$ with [(recall R, \dots are the weights and a, \dots the abscissae)]

$$Ra^m + R'a'^m + \text{etc.} + R^{(n)}a^{(n)m} = \frac{1}{m+1} - k^{(m)}.$$

Multiply by t^{m-1} and sum to get:

$$\frac{R}{t-a} + \text{etc.} + \frac{R^{(n)}}{t-a^{(n)}} = t^{-1} + \frac{1}{2}t^{-2} + \frac{1}{3}t^{-3} + \text{etc.} - \theta,$$

with

$$\theta = kt^{-1} + k't^{-2} + k''t^{-3} + \text{etc.}$$

($k, k', \text{ usque } k^{(n)}$ evanescere debere).

[The sequences of true values of the integral —*ie moments*— $1/(m + 1)$, approximate values $Ra^m + R'a'^m + \dots$ and errors $k^{(m)}$ are represented here by their Z-transforms or generating functions $\sum t^{-(m+1)}/(m + 1)$, \dots . These are the Cauchy transforms $\int_{-\infty}^{\infty} (t - x)^{-1} d\mu(x)$ of the true measure dx in $[0, 1]$, the measure $R\delta_a + R'\delta_{a'} + \dots$ associated with the quadrature rule and the difference between both.]

[Note ‘natural’ occurrence of the series $t^{-1} + \frac{1}{2}t^{-2} + \frac{1}{3}t^{-3} + \dots$ etc., which appeared above like *deus ex machina*.]

- Now recall $T(t^{-1} + (1/2)t^{-2} + \text{etc.}) = T' + T''$ to write

$$T \left(\frac{R}{t-a} + \frac{R'}{t-a'} + \text{etc.} + \frac{R^{(n)}}{t-a^{(n)}} \right) = T' + T'' - T\theta.$$

- *Pars prior ... est function integra ... ordinis n* whose values at a, a', \dots , are $MR, M'R', \dots$, i.e. those of T' . So left-hand side is T' .

- Hence we obtain the important relation

$$T'' = T\theta.$$

Therefore the error coefficients may be computed from the expansion of T''/T .

- If $y = K + K't + K''tt + \text{etc.}$, the error in $\int y dt$ will be $k^{(n+1)}K^{(n+1)} + k^{(n+1)}K^{(n+1)} + \text{etc.}$ [Gauss can't write reminder of Taylor polynomial.]

§15 to §16 (pages 24–26): main idea

- For any values of a, a', \dots , the formula obtained is exact for degrees $\leq n$.
- But for some values of a, a', \dots , the formula may be exact for higher degrees, as shown by the Cotes case with n even [something Gauss has discussed in detail in §6].
- For higher order we need to successively annihilate the error coefficients $k^{(n+1)}, k^{(n+2)}, \dots$ (coefficients of $t^{-n-2}, t^{-n-3}, \dots$ in θ). [i.e. it is a matter of $\theta = T''/T = (t^{-1} + \frac{1}{2}t^{-2} + \dots) - T'/T$ being 'small' at $t = \infty$.]

- Equivalently, we need to successively annihilate the coefficients of t^{-1} , t^{-2} , \dots in $T\theta$ i.e. in T'' . [Recall these are linear in α , α' , \dots , hence the advantage in multiplying by T .]
- *Since we have $n + 1$ free coefficients α , α' , \dots , we may annihilate the $n + 1$ leading coefficients of T'' and achieve degree $2n + 1$.*

[Writing $T(t) \int_0^1 \frac{dx}{t-x} = \int_0^1 \frac{T(t)-T(x)}{t-x} dx + \int_0^1 \frac{T(x)dx}{t-x}$, we see that $T' = \int_0^1 \frac{T(t)-T(x)}{t-x} dx$, $T'' = \int_0^1 \frac{T(x)dx}{t-x}$. After expansion,

$$T'' = t^{-1} \int_0^1 T(x)dx + t^{-2} \int_0^1 xT(x)dx + \dots$$

Thus annihilation of coefficients of T'' is equivalent to orthogonality of $T(x)$ to $1, x, \dots$]

- When the auxiliary variable u is used in lieu of t one has to approximate the function

$$\varphi = u^{-1} + \frac{1}{3}u^{-3} + \frac{1}{5}u^{-5} + \text{etc.}$$

by U'/U rather than $t^{-1} + \frac{1}{2}t^{-2} + \text{etc.}$ by T'/T .

- In the simplest example, $n = 0$, *coefficient unicus* of t^{-1} in *producto* $(t + \alpha)(t^{-1} + \frac{1}{2}t^{-2} + \frac{1}{3}t^{-3} + \text{etc.})$ *evanescere debet*. As this is $\frac{1}{2} + \alpha$, we have $\alpha = -\frac{1}{2}$ or $T = t - \frac{1}{2}$. [Midpoint rule.]

- The cases $n = 1$ and $n = 2$ (two and three linear equations to solve) also presented in detail; both in terms of t and u .

[Note it is assumed without proof that the linear system for the coefficients of T has a unique solution. Also assumed that T found in this way has distinct real roots.]

- But this way, *qui calculos continuo molestiores adducit, hic ulterius non persequemur, sed ad fontem genuinum solutionis generalis progrediemur.*

§17 to §21 (pages 26–36): a better way

- [Relating continued fractions and series.] *Proposita*

$$\varphi = \frac{v}{w + \frac{v'}{w' + \frac{v''}{w'' + \text{etc.}}}}$$

formentur duae quantitatum series $V, V', \text{ etc. } W, W', \text{ etc.}$

$$V = 0$$

$$W = 1$$

$$V' = v$$

$$W' = wW$$

$$V'' = w'V' + v'V$$

$$W'' = w'W' + v'W$$

$$V''' = w''V'' + v''V'$$

$$W''' = w''W'' + v''W'$$

etc. [Note three term recursions!]

- Then [quotients provide the convergents of the cted. fraction]

$$\begin{aligned} \frac{V}{W} &= 0 \\ \frac{V'}{W'} &= \frac{v}{w} \\ \frac{V''}{W''} &= \frac{v}{w + \frac{v'}{w'}} \\ \frac{V'''}{W'''} &= \frac{v}{w + \frac{v'}{w' + \frac{v''}{w''}}} \end{aligned}$$

and so on.

- [Fraction rewritten as series.] In addition, in the series

$$\frac{v}{W W'} - \frac{v v'}{W' W''} + \frac{v v' v''}{W'' W'''} - \frac{v v' v'' v'''}{W''' W^{iv}} + \text{etc.}$$

$$\textit{terminum primum} = \frac{V'}{W'}$$

$$\textit{summam duorum terminum primorum} = \frac{V''}{W''}$$

$$\textit{summam trium terminum primorum} = \frac{V'''}{W'''}$$

and so on. Similarly we represent *differentia inter* φ and $\frac{V'}{W'}$, $\frac{V''}{W''}$, etc.

[Recall that in terms of the auxiliary variable u the aim is to approximate by a rational function U'/U (U of degree $n + 1$, U' of degree n) the series

$$\varphi = u^{-1} + \frac{1}{3}u^{-3} + \frac{1}{5}u^{-5} + \text{etc.}]$$

• *E formula 33 Disquisitionum generalium circa seriem infinitam . . .*, [on the hypergeometric series (1812)] we transform φ into

$$\begin{array}{r}
 1 \\
 \hline
 u - \frac{\frac{1}{3}}{\frac{2 \cdot 2}{3 \cdot 5}} \\
 \quad u - \frac{\frac{3 \cdot 3}{5 \cdot 7}}{\frac{4 \cdot 4}{7 \cdot 9}} \\
 \quad \quad u - \frac{7 \cdot 9}{u - \text{etc.}}
 \end{array}$$

• Here $v = 1$, $v' = -\frac{1}{3}$, $v'' = -\frac{4}{15}$, etc. and $w = w' = w''$ etc. $= u$.

• So $W = 1$, $W' = u$, $W'' = uu - \frac{1}{3}$, $W''' = u^3 - \frac{3}{5}u$, etc.

[These are the monic Legendre polynomials, generated from the three term recursion!]

• And $V = 0$, $V' = 1$, $V'' = u$, $V''' = uu - \frac{4}{15}$, etc. [The associated polynomials of the three term recursion!]

- If $\varphi = \frac{V^{(m)}}{W^{(m)}}$ in *seriem descendente* convertitur, the first term is

$$\frac{2 \cdot 2 \cdot 3 \cdot 3 \cdots m \cdot m u^{-(2m+1)}}{3 \cdot 3 \cdots (2m-1)(2m-1)}.$$

[In modern terminology, $\frac{V^{(m)}}{W^{(m)}}$ is the Padé approximation to φ of degree $(m-1, m)$.] Thus if we set $U = W^{(n+1)}$ then $U\varphi$ is free of the powers $u^{-1}, \dots, u^{-(n+1)}$.

- Therefore the abscissas have to be chosen as the roots of the equation $W^{(n+1)} = 0$. [Zeros of Legendre polynomial.]

Next Gauss:

- Provides a closed form expression for the monic Legendre polynomials and discusses the relation to the hypergeometric function.
- Presents similar analysis for t in lieu of u . [T is of course the Legendre polynomial shifted to $[0, 1]$.]
- Gives explicit expression for the polynomial that yields the weights.

[The relation

$$T' = \int_0^1 \frac{T(t) - T(x)}{t - x} dx$$

we found before (resp. the corresponding formula that expresses U' in terms of U) is the well-known formula that relates the associated (or numerator) polynomials to the shifted Legendre polynomials T (resp. Legendre polynomials U). I am thankful to F. Marcellán for this observation.]

§22 to §23 (pages 36–40): using the rules

- For $n = 0, \dots, 6$ (one to seven nodes). Gauss provides:
 1. Polynomials U, U', T, T' .
 2. Abscissas a, a', \dots with 16 significant digits.
 3. Weights R, R', \dots with 16 significant digits. (For $n \geq 3$ also decimal logarithm with 10 significant digits.)
 4. The polynomial that gives the weights.
 5. The leading coefficient of the expansion of the error.

- *Methodi nostrae efficaciam ab oculis ponemos computando valores integralis $\int \frac{dx}{\log x}$ ab $x = 100000$ usque ad $x = 200000$ with rules with 1 to 7 nodes: (Bessel had computed 8406.24312)*

8390.394608

8405.954599

8406.236775

8406.242970

8406.243117

8406.243121

8406.2431211

[There are 8392 prime numbers in the interval.]