## Numerical integration over bounded intervals

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### Purpose

The purpose it to provide some basics on numerical integration over bounded intervals, that is

- description of symbolic software for computation of integrals;
- introduce the basic ideas on univariate polynomial interpolation;
- show some rules of interpolatory type, in the Newton-Cotes family, as midpoint, trapezoidal and Cavalieri-Simpson rules;
- disadvantages of Newton-Cotes rules and pros of composite rules;
- practical examples in Matlab/Octave.

The purpose is to compute

$$\int_{a}^{b} f(x) dx$$

where f is typically continuous in the interval [a, b].

## Numerical integration over bounded intervals

#### Remark

There are of course more general instances, e.g. f could have a finite number of jump discontinuities, but we will not take this case into account.

## Remark (Pathological continuous functions)

Between the continuous functions there are many odd examples, as the Weierstrass function

$$f(x) = \sum_{k=1}^{+\infty} \frac{\sin(\pi k^2 x)}{\pi k^2}$$

that is continuous everywhere but differentiable only on a set of null measure (proof by Hardy).

Poincaré defined it as "an outrage against common sense" and Hermite as a "lamentable scourge".

## Numerical integration over bounded intervals

- Analitically, a typical approach is to primitive) of the integrand.
- In view of the fundamental theorem of calculus (known as Torricelli-Barrow theorem), once a primitive is available then one can easily compute the definite integral.
- Unfortunately in many cases there are no known primitives in terms of elementary functions and one cannot adopt the technique described above.

## Function with no primitive in terms of elementary functions

Some examples of integrands with no primitive in terms of elementary functions, we have:

■ the function  $g: \mathbb{R} \to \mathbb{R}$  defined as

$$g(x) = \exp(x^2)$$

 $\blacksquare$  the function sinc :  $\mathbb{R} \to \mathbb{R}$  defined as

$$\operatorname{sinc}(x) = \begin{cases} \frac{\sin(\pi t)}{\pi t}, & x \neq 0, \\ 1, & x = 0 \end{cases}$$

The proof concerning the absence of primitives in terms of elementary functions depend on the Liouville theorem.

There are several environments for symbolic calculus, that allow the computation of definite and indefinite integrals, e.g.

- Maple, offering also online services;
- Mathematica, offering also online services;
- Maxima, free, with interesting online demo.

We will propose some examples to understand their usage.

As first example we consider a rational function and its integration that can be done by decomposition in partial fractions.

$$\int \frac{1+x-x^2}{1+x^2} dx = \frac{\log(x^2+1)}{2} - x + 2\arctan(x) + C$$

This technique has been discovered indipendently by Johann Bernoulli and Gottfried Leibniz (1702) and usually requires some boring computations.

2 As second example we consider  $\exp(-x^2)$ .

For each of them we will compute definite integrals in [0,1].

We first use Maple via Matlab shell for the computation of indefinite integrals.

```
>> svms x;
\Rightarrow int((1+x-x^2)/(1+x^2),x)
ans =
log(x^2 + 1)/2 - x + 2*atan(x)
>> int(exp(-x^2))
ans =
(pi^{(1/2)}*erf(x))/2
>> help erf
erf Error function.
    Y = erf(X) is the error function for each element of X. X must be
    real. The error function is defined as:
      erf(x) = 2/sqrt(pi) * integral from 0 to x of exp(-t^2) dt.
    See also erfc, erfcx, erfinv, erfcinv.
    Documentation for erf
    Other uses of erf
>>
```

Figure: Indefinite integrals in Maple (via Matlab shell).

Now we adopt Maple via Matlab shell for the computation of definite integrals.

```
\rightarrow int((1+x-x^2)/(1+x^2),0,1)
ans =
pi/2 + log(2)/2 - 1
>> format long
>> pi/2 + log(2)/2 - 1
ans =
   0.917369917074869
>> int(exp(-x^2),0,1)
ans =
(pi^(1/2)*erf(1))/2
>> (pi^(1/2)*erf(1))/2
ans =
   0.746824132812427
>>
```

Figure: Definite integrals in Maple (via Matlab shell).

We now make the computations of indefinite integrals via Mathematica, e.g. visiting the website Online Integral Calculator. To complete the computations, use the "equal "symbol on the right.



Figure: Indefinite integrals in Mathematica (via Online Integral Calculator).

About the second integral, we insert the new integrand and digit =on the right side of the box.



Figure: Indefinite integrals in Mathematica (via Online Integral Calculator).

Concerning definite integrals, writing the data in Math Input, clicking on *more digits*:



Figure: Definite integrals in Mathematica (via Online Integral Calculator).

We repeat the procedure for the second function.



Figure: Definite integrals in Mathematica (via Online Integral Calculator).

We repeat the computation by means of Maxima demo homesite

ntegrate	((1+x-x^2)/(1+x^2), x);			
Clic	Clear			
(%i1)	integrate((1	+x-x^2)	/(1+x^2),	x);
(%o1)	$\frac{\log(x^2+1)}{2} + 2 \arctan$	an x - x		

Figure: Indefinite integrals in Maxima (via online site).

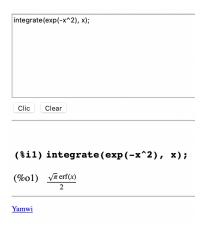


Figure: Indefinite integrals in Maxima (via online site).

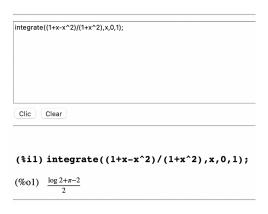


Figure: Definite integrals in Maxima (via online site).

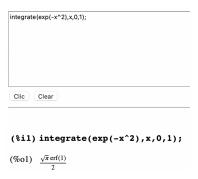


Figure: Definite integrals in Maxima (via online site).

#### Remark

The installation of Maxima may be not trivial (e.g. is not immediate on MacOS).

The previous definite integrals

$$\int_0^1 \frac{1+x-x^2}{1+x^2} dx \approx 0.917369917074869$$

$$\int_0^1 \exp(-x^2) dx \approx 0.746824132812427$$

may also be approximate by Matlab/Octave.

- We make the experiments in Octave, taking into account that the Matlab version is equal.
- To this purpose one can use OctaveOnline as well as Octave/Matlab.

## Adaptive codes in Matlab/Octave

We show how we can compute definite integrals in Matlab/Octave by adaptive algorithm implemented in integral, controlling the absolute and relative error, with tolerances decided by the users. This is guaranteed numerically but not mathematically (the code may fail in special and rare examples).

Consider that the function definition in Matlab/Octave requires the knowledge of pointwise operations, using ".".

```
>> f=@(x) (1+x-x.^2)./(1+x.^2);

>> Q = integral (f,0,1,'AbsTol',10^(-12),'RelTol',10^(-12));

>> Q

Q = 0.917369917074869

>> g=@(x) exp(-x.^2);

>> Q = integral (g,0,1,'AbsTol',10^(-12),'RelTol',10^(-12));

>> Q

Q = 0.746824132812427

>> |
```

Figure: Definite integrals in Octave.

## Univariate polynomial interpolation (summary)

#### Problema. (Univariate polynomial interpolation)

Given

- $\blacksquare$  n+1 distinct points  $x_0,\ldots,x_n$ ,
- the valuea  $y_0, \ldots, y_n$

the problem of polynomial interpolation consists in computing

$$p_n(x) = a_0 + \ldots + a_n x^n$$

such that

$$p_n(x_i) = y_i, i = 0, ..., n.$$

#### Example (Straight line for two given points)

Given 2 distinct points  $x_0, x_1$  and the values  $y_0, y_1$ , determine  $p_1 \in \mathbb{P}_1$  such that

$$p_1(x_0) = y_0, \quad p_1(x_1) = y_1$$
 (1)

that is the straight line that *passes* for the couples  $(x_0, y_0)$ ,  $(x_1, y_1)$ .

## Univariate polynomial interpolation (summary)

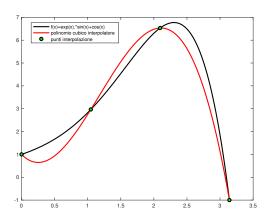


Figure: Example consisting in interpolating the function  $f(x) = \exp(x)\sin(x) + \cos(x)$  (in black) by an algebraic polynomial of degree 3 (in red) in 4 equispaced points in  $[0,\pi]$  (green circles). We plot the pertinent plots and the points  $\{(x_k,y_k)\}_{k=0,\dots,3}$ , where  $x_k=k\pi/3$  e  $y_k=f(x_k), k=0,\dots,3$ .

## Theorem (Existence and uniqueness of polynomial interpolant)

Given n+1 distinct points  $x_0, x_1, \ldots, x_n$  and the values  $vy_0, y_1, \ldots, y_n$ , the polynomial  $p_n \in \mathbb{P}_n$  such that

$$p_n(x_i) = y_i, \quad i = 0, \ldots, n.$$

exists and is unique.

Next

$$p_n(x) = \sum_{k=0}^n y_k L_k(x) = y_0 L_0(x) + y_1 L_1(x) + \ldots + y_n L_n(x)$$

where

$$L_k(x) := \prod_{j=0, j\neq k}^n \frac{x-x_j}{x_k-x_j} = \frac{(x-x_0)\dots(x-x_{k-1})(x-x_{k+1})\dots(x-x_n)}{(x_k-x_0)\dots(x_k-x_{k-1})(x_k-x_{k+1})\dots(x_k-x_n)}$$

is the k-th Lagrange polynomial w.r.t. the nodes  $\{x_k\}_{k=0,\ldots,n}$ .

The Lagrange polynomials where discovered by

- Waring in Problems concerning interpolations in 1779,
- rediscovered by Euler in 1783,
- published by Lagrange in Leçon Cinquième. Sur l'usage des courbes dans la solution des problèmes in 1795 (volume 7, p.286).

For an interesting note see A Chronology of Interpolation: From Ancient Astronomy to Modern Signal and Image Processing.

[ co ]

VII. Problems concerning Interpolations. By Edward Waring, M. D. F. R. S. and of the Inflitute of Bononia, Lucalian Professor of Mathematics in the University of Cambridge.

Read 10- 3. M.R. BRIGOS WAR the first perfon, I believe, 1779.

That invented a method of differences for interpolating logarithms at finall intervals from each other; his principles were followed by RRIFINATE and SOUTON in France. Sit PRACE XEWTON, from the fame principles, differenced a general and eagent follution of the abovementioned problem: perhaps a fiftil more eigenat one on fiome accounts has been finer different former fo

THEOREM I.

Affume an equation  $a+bx+cx^2+dx^3$ , ...,  $x^{n-1}=y_s$  in which the co-efficients a, b, c, d, e, &cc. are invariable;

1 2

66 Dr. WARING on Intertolations. x-xx-8×x-2×x-1×&c x-0×x-7×x-7×x-1×&c.  $\frac{1}{\beta-\alpha\times\beta-\gamma\times\beta-\delta\times\beta-1\times\delta c}$ , c= --×γ-β×γ-∂×γ-,×δα.  $\mathbf{p} = \frac{\mathbf{x} - \mathbf{x} \times \mathbf{x} - \beta \times \mathbf{x} - \gamma \times \mathbf{x} - i \times \delta \mathbf{c}_{\mathbf{c}_{\mathbf{c}}}}{\mathbf{x} - \mathbf{x} \times \mathbf{x} - \beta \times \delta - \gamma \times \mathbf{x} - i \times \delta \mathbf{c}_{\mathbf{c}_{\mathbf{c}}}}, \quad \mathbf{E} = \frac{\mathbf{x} - \mathbf{x} \times - \beta \times \mathbf{x} - \gamma \times \mathbf{x} - \delta \times \delta \mathbf{c}_{\mathbf{c}_{\mathbf{c}}}}{\mathbf{c} - \mathbf{x} \times \mathbf{x} - \beta \times \delta \times \mathbf{x} - \gamma \times \mathbf{x} - \delta \times \delta \mathbf{c}_{\mathbf{c}_{\mathbf{c}}}},$ &c.: fubftitute thefe values for A, B, C, D, E, &c. refpectively in the preceding equations (A+B+C+D+E+&c.=1.  $A\alpha + B\beta + C\alpha + D\beta + Ez + &C = x$ ,  $A\alpha^2 + B\beta^3 + C\alpha^3 + D\beta^3 +$  $E e^{3} + 8cc = x^{3}$ ,  $A \alpha^{3} + B \beta^{3} + C \gamma^{3} + D \delta^{3} + E e^{3} + 8cc = x^{3}$ , 8cc.) and there refult the equations (1)  $\frac{x-\beta \times x-y \times x-\delta \times x-z \times bc}{x-\beta \times x-y \times x-z \times bc}$  $\frac{x-a\times x-y\times x-\delta\times x-1\times\delta x_0}{\beta-a\times\beta-y\times\beta-\delta\times\beta-1\times\delta x_0} + \frac{x-a\times x-\beta\times x-\delta\times x-\delta\times x-y\times\delta x_0}{y-a\times y-\beta\times y-\delta\times y-\delta\times y-1\times\delta x_0} + &c. = 1;$  $(2) \alpha \times \frac{x - \beta \times x - \gamma \times x - \delta \times x - 1 \times \delta c}{x - \beta \times x - \gamma \times x - \delta \times x - 1 \times \delta c} + \beta \times \frac{x - x \times x - \gamma \times x - \delta \times x - 1 \times \delta c}{\beta - x \times \beta - \gamma \times \beta - \delta \times \delta - 1 \times \delta c}$  $+\gamma \times \frac{\overline{x-a \times x-\beta \times x-\beta \times x-\beta \times x-i} \times \delta c}{y-a \times y-\beta \times y-i \times y-i \times \delta c} + &c. = x;$  $(3)\alpha' \times \frac{x-\beta \times x-\gamma \times x-\delta \times x-x \times x_c}{\alpha-\beta \times \alpha-\gamma \times \alpha-\delta \times x-\delta \times x-x} + \beta' \times \frac{x-\alpha \times x-\gamma \times x-\delta \times x-x \times x_c}{\beta-\alpha \times \beta-\gamma \times \beta-\delta \times \beta}$ +  $\gamma^s \times \frac{x - s \times x - \beta \times x - \gamma \times x - r \times \delta cc}{y - s \times \gamma - \beta \times y - \delta \times \gamma - r \times \delta cc}$  =  $x^s$ ; and in general,  $\alpha^{m} \times \frac{x - \beta \times x - \gamma \times x - \delta \times x - \gamma}{\alpha - \beta \times x - \gamma \times x - \delta \times x - x} e_{c.} + \beta^{m} \times \frac{x - \alpha \times x - \gamma}{\beta - \alpha \times \beta - \gamma \times \beta - \delta \times x} e_{c.} \times \delta c.$  $+\gamma^m \times \frac{x-a \times x-\beta \times x-\delta \times x-i \times bc}{y-a \times \gamma-\beta \times \gamma-i \times \gamma-i \times bc} + \delta^m \times \frac{x-a \times x-\beta \times x-\gamma \times x-i \times bc}{\delta-a \times \delta-\beta \times \delta-\gamma \times \delta-i \times bc}$ +8cc.=xm, whatever may be the values of the quantities x; α, β, γ, δ, ε, &cc.: reduce all these fractions into terms. proceeding according to the dimensions of the quantity x, and it is evident, that the fum of all the fractions multiplied

Figure: The paper by Waring in which the Lagrange polynomials were discovered.

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# DE EXIMIO VSV METHODI INTERPOLATIONVM IN SERIERVM DOCTRINA.

In methodo interpolationum elusmodi relatio inter binas variabiles x et y quaeritur, vt fi alteri x successine dati valores a, b, c, d, etc. tribuantur, altera y inde quoque datos valores p, q, r, s, etc. forciatur; feu quod codem redit, acquatio pro ciusmodi linea curua quaeritur, onae per quotcunque puncta data transeat. Ono major ergo fuerit horam punctorum numerus, co magis linea curua limitatur; interim tamen iam alia occasione observani, etiamfi punctorum numerus in infinitom augeatur, curuam per ea tranfeuntem non prorius determinari, fed femper infinitas adhuc lineas curuas exhiberi posse, quae seque per cuncta cadem puncta fint transiturae. Quare cum methodus interpolationum pro quonis casa lineam curuam suppediter determinatum, folutio haec semper pro maxime particulari erit habenda: verum haec ipfa circumfrantia fineularem quandam indolem folutionis inventae innuit, quae accuratiorem confiderationem meretur. Imprimis autem itla folutionis indoles pendet a ratione, qua interpolatio inflituitur, feu a forma, quae acquationi generali tribultur, in qua acquationem quaesitam contineri

Figure: Paper by Eulero in which the Lagrange polynomials were rediscovered.

#### 286 LEÇONS ÉLÉMENTAIRES

qu'en faisant x = p on ait

$$A = r$$
,  $B = o$ ,  $C = o$ , ...;

que de même, en faisant x = q, on ait

$$A = 0$$
,  $B = 1$ ,  $C = 0$ ,  $D = 0$ , ...;

qu'en faisant x = r, on ait pareillement

$$A = o$$
,  $B = o$ ,  $C = i$ ,  $D = o$ , ..., etc.;

d'où il est facile de conclure que les valeurs de A, B, C, . . . doivent être de cette forme

$$\begin{split} \mathbf{A} &= \frac{(x-q)\left(x-r\right)\left(x-s\right)\dots}{(p-q)\left(p-r\right)\left(p-s\right)\dots},\\ \mathbf{B} &= \frac{(x-p)\left(x-r\right)\left(x-s\right)\dots}{(q-p)\left(q-r\right)\left(q-s\right)\dots},\\ \mathbf{C} &= \frac{(x-p)\left(x-q\right)\left(x-s\right)\dots}{(r-p)\left(r-q\right)\left(r-s\right)\dots}, \end{split}$$

Figure: Work by Lagrange on the relative polynomials.

## Choice of interpolation points

One may believe that if we take more and more equispaced nodes in [a, b], that is

$$x_k = a + k \frac{(b-a)}{n}, \ k = 0, \dots, n$$

increasing n, the polynomial  $p_n$  will approximate better and better the function f, but it is not so.

Runge discovered a famous counterexample in Über die Darstellung willkrlicher Functionen und die Interpolation zwichen äquidistanten Ordinaten, p.243, (1901), that is  $f \in C^{\infty}([-5,5])$  defined by

$$f(x) = \frac{1}{1+x^2}, \ x \in [-5, 5]$$

in which increasing n,  $\max_{x \in [a,b]} |f(x) - p_n(x)|$  does not converge to 0.

## Runge counterexample

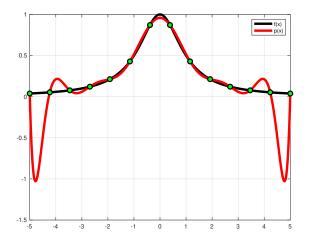


Figure: Plot illustrating the polynomial interpolant (of the Runge function) of degree 12 based on 13 equispaced nodes. The plot in red is the interpolant, while the plot in black is the Runge function. The green dots are the couples to be interpolated. Observe the wild obscillations at extrema. Increasing the degree

## Runge counterexample

#### Über empirische Funktionen und die Interpolation zwischen äquidistanten Ordinaten.

Von C. RUNGE in Hannover.

Die Abhängigkeit zwischen zwei messbaren Grössen kann, strenge genommen, durch Beobachtung überhaupt nicht gefunden werden. Denn selbst wenn man von den Beobschtungsfehlern absehen und die Beobachtungen als absolut genau voraussetzen wollte, so bliebe doch immer der Umstand, dass durch Beobachtung immer nur eine diskrete Reihe einander entsprechender Wertepaare der beiden Grössen gefunden werden könnte. Selbst wenn wir die Reihe als unendlich vorsus setzten, so würde nicht einmal eine "analytische"1) Funktion dadurch bestimmt sein. Gesetzt z. B., es seien für eine unendliche Reihe von äquidistanten Werten der einen Grösse die Werte der andern Grösse absolut genau bekannt, so wäre das Abhängigkeitsverhältnis damit noch nicht gegeben, selbst dann nicht, wenn wir nur nach der "analytischen" Funktion fragen, die das Abhängigkeitsverhältnis darstellen soll. Denn es ist klar, dass man auf mannigfache Weise eine periodische Funktion bilden kann, die für alle iene äquidistanten Werte verschwindet und daher, zu einer Funktion addiert, ihre Werte an jenen Stellen nicht ändert. Dennoch betrachtet man in den beobachtenden Wissenschaften eine Funktion durch eine solche Tabelle ihrer Werte als wohl definiert, sobald die Argumente nur hinreichend nahe aneinander liegen. Wie dicht sie liegen müssen, darüber werden meines Wissens klare Kriterien nicht aufgestellt. Man beschränkt sich darsuf zu verlangen, dass die beobachteten Werte graphisch aufgetragen eine "glatte Kurve" geben. Eine Wellenlinie, die zwischen ie zwei aufeinanderfolgenden beobachteten Punkten ein Maximum oder Minimum hätte, würde man stillschweigend ausschliessen.

Dieses übliche Verfahren kann in der That auch mathematisch gerechtfertiet werden.

Man kann nämlich auch durch eine Tabelle eine Funktion wohl definieren, wenn man zugleich ein Interpolationsverfahren vorschreibt. Von C. Rainge. 243

Es sei z. B.  $f(x) = \frac{1}{1+x^4}$  und a=-5, b=+5. Dann hat f(x) die beiden singulären Stellen +i und -i. Statt eines Kreises haben wir dann zwei Kreise auszuschliessen und erhalten, wenn wir die U-Kurve in Zunendliche Ticken lassen

Wird daher n als ungrade vorausgesetzt, so muss  $g_n(i)$  rein imaginär sein:  $g_n(i) \ = \pm \ i \mid g_n(i) \mid$ 

und wir erhalten:  

$$\frac{g_n(-i) - \frac{1}{\pi i} |g_n(i)|}{1 + x^i} = G_n(x) \pm \frac{g_n(x)}{|g_n(i)|} \frac{x}{1 + x^i}.$$

<sup>1)</sup> Im Sinne von Weierstrass.

Figure: Original paper on Runge counterexample.

## Interpolatory qaudrature rules

The following theorem holds.

## Theorem (Stability of integration)

If  $\tilde{f}, f \in C([a,b])$ , and [a,b] is a bounded interval then

$$\left| \int_a^b f(x) dx - \int_a^b \tilde{f}(x) dx \right| \leq (b-a) \max_{x \in [a,b]} |f(x) - \tilde{f}(x)|.$$

Thus, if we assume that

- the points  $\{x_k\}_{k=0,...,n} \subset [a,b]$  are distinct,
- the polynomial  $\tilde{f} = p_n$  that interpolates  $(x_0, f(x_0)), \dots, (x_n, f(x_n))$  is a *good* approximation of  $f \in C([a, b])$ .

then

$$I(p_n) = \int_a^b p_n(x) dx \approx I(f) = \int_a^b f(x) dx$$

with the advantage that the computation of  $I(p_n)$  is usually easier than that of I(f).

## Interpolatory quadrature rules

In virtue of what we have seen, let  $L_k$  be the Lagrange polynomials relatively to the set  $\{x_k\}_{k=0,\dots,n}$ , and the weights

$$w_k = \int_a^b L_k(x) dx$$

and get

$$\int_{a}^{b} f(x)dx \approx \int_{a}^{b} p_{n}(x)dx = \int_{a}^{b} \sum_{k=0}^{n} f(x_{k})L_{k}(x)dx$$

$$= \sum_{k=0}^{n} \int_{a}^{b} f(x_{k})L_{k}(x)dx = \sum_{k=0}^{n} f(x_{k}) \int_{a}^{b} L_{k}(x)dx$$

$$= \sum_{k=0}^{n} w_{k}f(x_{k}).$$

that is

$$\int_a^b f(x)dx \approx \sum_{k=0}^n w_k f(x_k).$$

(2)

## Interpolatory quadrature rules

Observe that if  $f \in \mathbb{P}_n$  then it it is exactly the polynomial  $p_n$  that interpolates the couples  $(x_k, f(x_k))$ ,  $k = 0, \dots, n$  (by the uniqueness of the polynomial interpolant) and then

$$\int_{a}^{b} f(x) dx = \int_{a}^{b} p_{n}(x) dx = \int_{a}^{b} \sum_{k=0}^{n} f(x_{k}) L_{k}(x) dx = \ldots = \sum_{k=0}^{n} w_{k} f(x_{k}).$$

Cnosequently, if  $f \in \mathbb{P}_n$  then  $\sum_{k=0}^n w_k f(x_k)$  is equal to  $\int_a^b f(x) dx$ .

We will say that the degree of exactness of an interpolatory rule in n + 1 nodes is at least n.

Thus, an interpolatory rule on

- 1 node, surely integrates exactly the constants;
- 2 nodes, surely integrates exactly the polynomials of degree 0, 1;
- 3 nodes, surely integrates exactly the polynomials of degree 0, 1, 2.

We will see that sometimes things can be even better.

## Interpolatory quadrature rules

The fact that

$$\int_a^b f(x)dx \approx \sum_{k=0}^n w_k f(x_k), \quad w_k = \int_a^b L_k(x)dx$$

says that to approximate the required integral it is not necessary to

- 1 compute the polynomial interpolant,
- 2 determine its primitive,
- 3 apply the fundamental theorem of integral calculus,

but

- compute the weights  $\{w_k\}_{k=0,...,n}$  relatively to the nodes  $\{x_k\}_{k=0,...,n}$ ,
- **2** use the function evaluations  $\{f(x_k)\}_{k=0,...,n}$ .

#### Remark

This fact is important, since if we change the integrand we minimize the computation, since the weights  $w_k$ ,  $k=0,\ldots,n$  do not change, depending only on the nodes.

## Rectangular rule

## Definition (Rectangular rule)

Let

- $f \in C([a, b]), -\infty < a < b < +\infty$ ,
- $x_0 \in [a, b]$ .

The rettangular rule is defined by

$$\int_{a}^{b} f(x)dx \approx w_{0}f(x_{0}) = (b-a)f(x_{0}) := S_{0}^{*}(f).$$
 (3)

If  $x_0 = \frac{a+b}{2}$  we get the so called midpoint rule.

## Midpoint rule

For the midpoint rule, the following error estimate holds

## Theorem (Midpoint rule error estimate)

If  $f \in C^{(2)}([a,b])$  then the midpoint rule error estimate is

$$E_0(f) := I(f) - S_0^*(f) = \frac{(b-a)^3}{24} f^{(2)}(\xi), \ \xi \in (a,b).$$

Observe that if  $f \in \mathbb{P}_1$  allora

$$E_0(f) := I(f) - S_0^*(f) = 0$$

thus the rule is exact.

This is a little surprising since being based on just one function evaluation one may believe it integrates exactly just the constants and not polynomials of degree 1.

## Rectangular rule

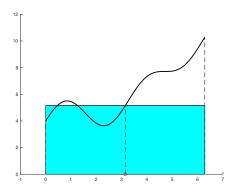


Figure: Rectangular rule with node  $x_0 = (a+b)/2$ , a=0,  $b=2\pi$ , for approximating  $\int_0^{2\pi} (3+\sin(2x)+\cos(x)+x) \, dx$  (midpoint rule computes the area in cyan).

# Trapezoidal rule.

### Definition (Trapezoidal rule)

The trapezoidal rule is defined by

$$\int_a^b f(x)dx \approx S_1(f) := \frac{b-a}{2} \cdot (f(a) + f(b)).$$

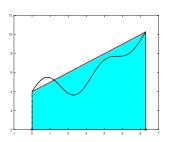


Figure: Trapezoidal rule for the approximation of  $\int_0^{2\pi} 3 + \sin(2x) + \cos(x) + x \, dx$  (the rule computes the area in cyan).

# Trapezoidal rule

# Theorem (Error of the Trapezoidal rule)

If  $f \in C^2([a,b])$  then the error of the trapezoidal rule is

$$E_1(f) := I(f) - S_1(f) = \frac{-(b-a)^3}{12} f^{(2)}(\xi), \ \xi \in (a,b).$$

# Theorem (Degree of exactness of the trapezoidal rule)

The degree of exactness of the trapezoidal rule is exactly 1.

# Definition (Cavalieri-Simpson rule)

The Cavalieri-Simpson rule is defined as  $\int_a^b f(x)dx \approx S_2(f)$  with

$$S_2(f) := \frac{b-a}{6} \cdot f(a) + \frac{2(b-a)}{3} \cdot f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} \cdot f(b).$$

This interpolatory rule is equivalent to determine the definite integral for the polynomial with nodes the interval extrema a, b and their midpoint (a + b)/2.

Consequently, its degree of exactness is at least 2.

# Cavalieri-Simpson rule

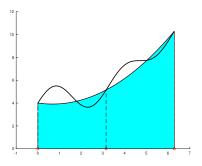


Figure: Cavalieri-Simpson rule for the computation of  $\int_0^{2\pi} 3 + \sin(2x) + \cos(x) + x \, dx$ , it determines the area in cyan).

# Cavalieri-Simpson rule

### Theorem (Cavalieri-Simpson rule error)

If  $f \in C^4([a,b])$  the error made by Cavalieri-Simpson rule is

$$E_2(f) := I(f) - S_2(f) = \frac{-h^5}{90} f^{(4)}(\xi), \quad h = \frac{b-a}{2}$$

with  $\xi \in (a, b)$ .

### Theorem (Degree of exactness of Cavalieri-Simpson rule)

The degree of exactness of Cavalieri-Simpson rule is exactly 3.

### Remark

As in the case of midpoint rule, this result is remarkable, since it is expected to be 2, since the formula of interpolatory type is based on 3 nodes.

Observe that integration had a complicated history.

Cavalieri did not have the modern concept of integration since he was researcher between 1629 and 1647, while

- the fundamental of integral calculus by (Torricelli-Barrow) appears in a primitive form in Lectiones geometricae by Barrow (1670) and in Geometriae pars universalis by Gregory (1668), see [?];
- Riemann integral was introduced in december 1853 (in his habilitation thesis);
- Lebesgue integral was discovered in 1904.

Cavalieri, by means of the so called method of indivisibles computed  $\int_a^b x^n dx$  for n = 1, ..., 9.

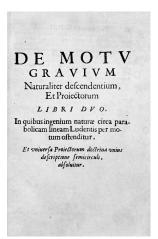


Figure: Work by Torricelli in which the fundamental theorem of integral calculus is introduced geometrically (link between displacement on a straight line and velocity).



#### LECTURE XI

Change of the independent variable in integration. Integration the inverse of differentiation. Differentiation of a quotient. Area and centre of gravity of a paraboliform. Limits for the are of a circle and a hyperbola. Estimation of \( \pi \).

#### Note

In the following theorems, Barrow uses his variation of the usual method of summation for the determination of an area. If ABKJ is the area under the curve AJ, he divides BK into an infinite number of equal parts and erects ordinates. In his figures he generally makes four parts

do duty for the infinite number.

He then uses the notation already mentioned, namely, that the area ABKJ is equal to the sum of the ordinates AB,

CD, EF, GH, JK.

The same idea is involved when he speaks of the sum of the rectangles of DD B, EF FD, GH FH, JK GH; for this sum, where commas are used between the quantities instead of a plus sign, does not stand for the area ABKd, but for where an ordinate HG is such that R HG and R is some given length; in other wore proportional to each of the rectangles are apply

between the quantities instead of a plus 8 0 P M w.
sign, does not stand for the area ABKJ, but for R ABKI,
where an ordinate HG is such that HG = HG is
not proportional to each of the rectungs of a population of
the line BK, and their aggregate or sum is found;
benece this sum is of three dimensions. On the contrary,
the uses the same phrase, with plus signs instead of commas,
to stand for a simple summation.

Figure: Work by Barrow in which a geometrical form of fundamental theorem of calculus. On this subject, see also the paper Barrow and Leibniz on the fundamental theorem of the calculus.

# GEOMETRIÆ PARS VNIVERSALIS, Inferviens Quantitatum Curvarum transmutationi & mensurz. AVTHORE IACOBO GREGORIO ABREDONENSI S C O T O. PATAVII, MDCLXVIII. Typis Heredum Pauli Frambotti, Superiorum Perm. CVM PRIVILEGIO.

Figure: Geometriae pars universalis, published in Padua in 1668.

#### Historical notes

At the webpage Riemann integral we find this interesting remark.

The Riemann integral was introduced in Bernhard Riemann's paper "Über die Darstellbarkeit einer Function durch eine trigonometrische Reihe" (On the representability of a function by a trigonometric series; i.e., when can a function be represented by a trigonometric series).

This paper was submitted to the University of Göttingen in 1854 as Riemann's Habilitationsschrift (qualification to become an instructor).

It was published in 1868 in Abhandlungen der Königlichen Gesellschaft der Wissenschaften zu Göttingen (Proceedings of the Royal Philosophical Society at Göttingen), vol. 13, pages 87-132.

For Riemann's definition of his integral, see section 4, "Über den Begriff eines bestimmten Integrals und den Umfang seiner Gültigkeit" (On the concept of a definite integral and the extent of its validity), pages 101–103.

### Historical notes



Figure: Monograph in which the Riemann integral was introduced.



Figure: Monograph in which the Lebesgue integral was introduced.

### Cavalieri-Simpson rule

About the ascription to Cavalieri, Peano wrote in Residuo in Formula de quadratura Cavalieri-Simpson (1916), in a simplified latin language, that this formula was discovered by Cavalieri (1639), Gregory (1668), Cotes (1722) and Simpson (1743).

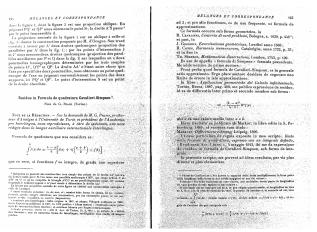


Figure: Peano paper and historical notes on the ascription of this rule.

# Cavalieri-Simpson rule

It is surprising why Cavalieri for what purpose Cavalieri used this rule.

At that time there were many efforts on solids of rotation. For instance, Kepler in Nova stereometria doliorum vinariorum that is *New measure of the volume of barrels of wine* justified an empirical method used by austrian coopers, by means of a geometrical approach.

Also Cavalieri had some interest on the topic. In Note - Postille Matematiche, Gabrio Piola, discusses of the work *Centuria di varii problemi*, by Cavalieri. In particular at page 83, he writes

Problem 80 concerns the measure of elliptical-circular barrels, giving a rule that is exactly the same that nowadays stems from Rossi-Amulis formula, demonstrated in 1806.

### Historical notes

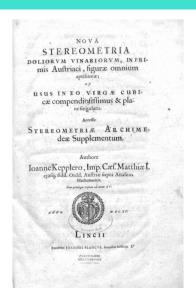


Figure: Cover of Kepler work *Nova stereometria doliorum vinariorum* on the volume of barrels.



Figure: The cover of the work by Cavalieri, suggested by Peano.

1 Phrasi de Cavalieri es « Per havere la capacità della botte moltiplicaremo la terza parte della lunghezza della botte in due cerchi maggiori ed uno dei minori ».

Versione « Pro habe capacitate de vase vinario, nos multiplica tercio parte de longitudine de vase per duo circulo maiore et uno minore ».

Si nos sume axi de vase pro axi de x, et pro origine puncto medio, si longitudine de vase es h, et si f(x) es area de sectione de vase, in puncto de abscissa x, et normale ad axi, tunc

volumine 
$$=\int_{-h/2}^{h/2} f(x) dx$$
; circulo maiore  $=f(0)$ , circulo minore  $=f(h/2)=f(-h/2)$ ; et re-

gula de Cavalieri dic que integrale vale :

$$\frac{h}{3} \left[ 2f(0) + f(h/2) \right] = \frac{h}{6} \left[ 4f(0) + f(-h/2) + f(h/2) \right].$$

Figure: Remark by Peano on the volume of barrels.

1948. In Vino Veritas:—"Si adunque moltiplicaremo la terza parte di *IM* lunghezza della Botte *BDFH* in due cerchi maggiore *CG* e uno de minore *BH*, *DF* come in *BH*, ci verrà la capacità di detta Botte." F B. Cavalieri, *Una centuria di varii Problemi nella Prattica Astrologica*, (Bologna, 1639), Problema 80. [Per Dr. G. N Watson. It was probably this formula for the capacity of a cask of wine which suggested to James Gregory (who spent the years 1665–8 in Padua) the more general formula for approximate integration, often written in the form

$$\int_0^{2h} y \, dx = h(y_0 + 4y_1 + y_2)/3,$$

which, in its turn, led to the outstanding generalisations due to Newton and Cotes, and subsequently to the minor generalisation known as 'Simpson's rule'; about this rule (published in 1743) there is not much to be said except that it is more accurate than the 'trapezoidal rule' ] [Per Dr. G N. Watson]

Figure: Remark by G.N. Watson about Cavalieri and the volume of barrels.

Problema 79. quello, the dimoftra Archim. ne Lib. de Sphæra, & Cylindro, perciò basta. rà misurare il cerchio di, BA, semidiametro, cioè giungeremo infieme il log. del cerchio della Tauoletta del Prob.66 che è 049715. con il doppio del log,di, BA, cioè con il log. di, EA, 130102.e di.AI,060206, (perche.E A, AB, AI, (ono proportionali) e ne verrà il logar.240024. di p.251.33.e tanto farà la superficie di detra portione di sfera. La scio poi l'Essempio per la folidirà della portione dello sferoide, non effendo diffimile l'operatione da quella della sfera.

#### PROBLEMA 80.

Misurare la capacità delle Botti.

S la di mono posta qua la figura del grob ant, mella quale fiano le due portioni, a B H, D E F, li cui assi, A I, M E, siano eguali, onde ti a le basi di quelle, cioètra li cerchi. B H, D F, che faranno eguali, resi compreso il corgo, po, o Botte, BDFH, e per, L. centro paff hG. G, diametro del cetchio maggiores C Gi, perpendicolare ad, AE.

Per hauere adun-

Per hauere adunque la capacità della Botte, B D FH, fi potria mifurare me-

dianti gli affi, AE, CG; cutto lo sferoide, ACEG, per il rolo, 77, e poi per il reol, ant. le due portioni, BAH; DE F, le quali fottratte dallo sferoide, A CEG, ci la foiariano la capacità della Botte, BDFH, ma perche quella della Botte, BDFH, ma perche quella della pollunga fattura, perciò ci potremo feruire di quelli altri modi, come più facili.

Se adunque moltiplicaremo la terza parte di, I M, lunghezza della Bote, B D F H, in due cerchi maggiori, CG, & vno de minori, BH, DF, come m, B H, ci verra la capacita di detta Botte. E peiò quadraremo il cerchio di, C G, in le ltc. F.

10.

Problema 80. 447 do nuono per 7854 e partendo il prodotto di nuono per 7854 e partendo il auuenimento per 10000 (che fono li termini della proportione del quadrato al cerchio inferitto) poiche il quotiente farà il cerchio, C G e così anco quadratemo il terzo di, I M, nelli due cerchi, CG, & vno, BH, e ne veri al a capacità della Bote, BDFH.

E per i log. giungendo infieme il log. della ter za parte disIMs-có il log. del cerchio o C G, cioè con il log. del cerchio della Tanoletta del prob. 66-che è 049715, e con il log. del prob. 66-che è 049715, e con il log. del prob. 66-che è 049715, e con il log. del Binario, ne verrà il log. di vin primo inoemo. Di poi giungendo parimente infieme il log. della terza parte disIMs-con il log. del cerchio, B H. cioè con il log. del cerchio della Tau. del Prob. 66-c con il log. duplicato di B Is. ne verrà il log. di vin fecondo inuento, il quale giunto al primo ci darà la capacità della Botte. B D F H.

ES-

#### Historical notes

The same rule can be found in Mathematical dissertations On A Variety of Physical and Analytical subjects by Thomas Simpson. It is clear that T. Simpson is thinking to composite rules.

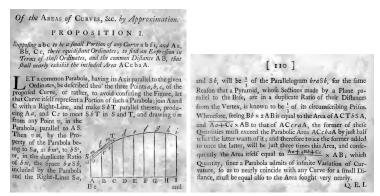


Figure: Excerpt from Mathematical dissertations On A Variety of Physical and Analytical subjects by T. Simpson.

### Considerazione.

Assume that  $f \in C([a,b])$ , where [a,b] is bounded.

By Weierstrass theorem, since that function can be approximated arbitrary well and uniformly by polynomials, one may believe that that rules with higher degree may approximate arbitrarialy well the definite integral, but we shall see this is not true.

After the previous note on Runge function, one forsees that if the nodes are  $\{x_k\}_{k=0,...,n}$  some problems may happen.

We will see later the results.

### Definition (Newton-Cotes rules)

Let [a, b] be a bounded interval. A rule

$$S_n(f) = \sum_{i=0}^n w_i f(x_i) \approx \int_a^b f(x) dx$$

is of closed Newton-Cotes type if

• that the set of nodes is equispaced and contains the extrema, that is

$$x_i = a + \frac{i(b-a)}{n}, i = 0, ..., n,$$

the weights are

$$w_i = \int_a^b L_i(x) dx, \ i = 0, \ldots, n, \ L_i(x) = \prod_{i=0, i \neq i}^n \frac{(x - x_i)}{x_i - x_i}.$$

# Remark (Degree of exactness of closed Newton-Cotes formulae)

This rule is interpolatory and has n + 1 nodes, thus it has degree of exactness at least n.

### Remark (Facoltativa)

- These rules were introduced by Newton in 1676 and described in Of Quadrature by Ordinates in 1695. The literature is not clear, it written they had 5 ordinates (so degree of exactness at least 4).
- Cotes, that was editor of the second version of the Principia, generalised the results by Newton, possibly in 1707, though they were published in 1722. In particular Cotes computed rules that had up to 11 nodes.

Considering Harmonia mensurarum, it is not easy to found where these rules are. An appendix is sometimes mentioned, but it is not easy to understand where it can be found.

Historians say that Cotes was not cited and paid for his work in the second version of Newton's Principia. In spite of that, when Cotes died at 34 yo, Newton said If he had lived, we might have known something.

# HARMONIA MENSURARUM, SIVE ANALYSIS & SYNTHESIS Per RATIONUM & ANGULORUM MENSURAS PROMOTÆ: ACCEDUNT ALIA OPUSCULA MATHEMATICA: PER ROGERUM COTESIUM. - Si propius stes, Te capient magis .-EDIDIT ET AUXIT ROBERTUS SMITH Collegii S. Trinitatis apud Cantabrigienses Socius; Aftronomiæ & Experimentalis Philosophiæ Post COTESIUM Professor. CANTABRIGIÆ, MDCCXXII.

Figure: First page of Harmonia mensurarum

#### Newton-Cotes rules

We show numerically the lack of convergence of the Newton-Cotes closed formula when applied to compute  $\int_{-5}^{5} 1/(1+x^2)dx$  (i.e. we adopt as integrand the RUnge function). Since the interpolant is far from approximating the Runge function we believe that also the integrals will be very different.

n	Integral Intp. Pol.	Absolute Error
1	3.846153846153846 <i>e</i> - 01	2.362e + 00
2	6.794871794871796 <i>e</i> + 00	4.048 <i>e</i> + 00
3	2.081447963800905 <i>e</i> + 00	6.654 <i>e</i> — 01
4	2.374005305039788 <i>e</i> + 00	3.728 <i>e</i> — 01
5	2.307692307692308 <i>e</i> + 00	4.391 <i>e</i> — 01
6	3.870448673470800 <i>e</i> + 00	1.124 <i>e</i> + 00
7	2.898994409748379 <i>e</i> + 00	1.522 <i>e</i> — 01
8	1.500488907127907 <i>e</i> + 00	1.246 <i>e</i> + 00
9	2.398617897841837 <i>e</i> + 00	3.482 <i>e</i> — 01
10	4.673300555653490 <i>e</i> + 00	1.926 <i>e</i> + 00
15	4.155558992699889 <i>e</i> + 00	1.409 <i>e</i> + 00
20	-2.684955208653064e + 01	2.960 <i>e</i> + 01

Table: Newton-Cotes formulas failing to approximate  $\int_{-5}^{5} 1/(1+x^2) dx \approx 2.746801533890032$ .

composite rules are obtained integrating a piecewise polynomial interpolant of degree m.

#### As example,

- we subdivide [a, b] in L equispaced intervals  $[t_0, t_1], \ldots, [t_{L-1}, t_L]$ ;
- define in each  $[t_{k-1}, t_k]$  a set of m+1 equispaced points  $x_{m(k-1)} < \ldots < x_{mk}$  con  $t_{k-1} = x_{m(k-1)}$  and  $t_k = x_{mk}$ ;
- let " $s_m$ " the piecewise polynomial interpolant of degree m, relatively to the subdivision  $[t_k, t_{(k+1)}]$ , with  $k = 0, \ldots, L$ , and couples  $(x_j, f(x_j))$ ,  $j = 0, \ldots, n = Lm$ ;
- suppose that  $S_m(f, t_{k-1}, t_k)$  is a closed formula of Newton-Cotes close type, in the interval  $[t_{k-1}, t_k]$ , with m+1 nodes (so having at least degree of exactness m).

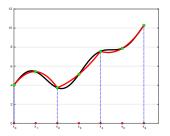


Figure: In black: the function  $f(x) = 3 + \sin(2x) + \cos(x) + x$ . In red: the piecewise interpolant  $s_m$  of degree m = 2, relatively to the subdivision  $[t_k = x_{2k}, t_{k+1} = x_{2(k+1)}]$ , with k = 0, 1, 2, and to the couples  $(x_j, f(x_j))$ ,  $j = 0, \ldots, n = 6$ . In green: the couples  $(x_i, f(x_j))$ ,  $j = 0, \ldots, 6$ .

# composite rules

- Being  $s_m$  a polynomial of degree m in each  $[t_k, t_{k+1}]$ ,
- since  $S_m(f, t_k, t_{(k+1)})$  has degree of exactness m,

by additivity of integration operator

$$\int_{a}^{b} f(x)dx \approx \int_{a}^{b} s_{m}(x)dx 
= \int_{t_{0}=a}^{t_{1}} s_{m}(x)dx + \int_{t_{1}}^{t_{2}} s_{m}(x)dx + \dots + \int_{t_{L-1}}^{x_{L}=b} s_{m}(x)dx 
= S_{m}(f, t_{0}, t_{1}) + S_{m}(f, t_{1}, t_{2}) + \dots + S_{m}(f, t_{L-1}, t_{L})$$

Thus we obtained the approximation of the integral not by a Newton-Cotes rule with high degree of exactness "n", but applying the same rule with a low ADE "m" in each subinterval, summing up all the contributions.

### Definition (Composite rule)

Let

- [a,b] a bounded interval,
- 2  $t_j = a + jh$  with h = (b a)/N, j = 0, ..., N,
- **3**  $S(f, \alpha, \beta)$ ) a rule in the bounded interval  $[\alpha, \beta]$ .

The quadrature formula

$$S^{(c)}(f, a, b, N) = \sum_{j=0}^{N-1} S(f, t_j, t_{j+1})$$
 (4)

è is a composite rule using S.

### Remark

In this discussion, the points  $x_j$ ,  $j=0,\ldots,N$ , will be equispaced, but with some effort we can extend the analysis to a different distribution. In other terms:

- if  $t_0 = a < t_1 < \ldots < t_N = b$ , one partitions [a, b] as union of subintervals  $[t_k, t_{k+1}], k = 0, \ldots, N-1$ ;
- in each subinterval we apply the same rule, summing up the contributions.

### Definition (Midpoint composite rule)

The midpoint composite rule is defined as

$$S_0^{(c)}(f, a, b, N) := \frac{b-a}{N} \sum_{k=0}^{N-1} f(x_k),$$
 (5)

where  $x_k$  is the midpoint of the k + 1-th interval, that is

$$x_k = a + \frac{2k+1}{2} \cdot \frac{b-a}{N}, k = 0, \dots, N-1.$$

Subdividing [a,b] in N equispaced interval  $[t_k,t_{k+1}]$ ,  $K=0,\ldots,N-1$  with  $t_j=a+jh,j=0,\ldots,N$ , h=(b-a)/N, if  $x_k$  is the midpoint of  $[t_k,t_{k+1}]$  then

$$x_k = \frac{t_k + t_{k+1}}{2} = \frac{a + kh + a + (k+1)h}{2} = a + \frac{(2k+1)h}{2}.$$

and since  $w_k = t_{k+1} - t_k = a + (k+1)h - (a+kh) = h = (b-a)/N$  we get

$$S_0^{(c)}(f, a, b, N) := \sum_{k=0}^{N-1} \frac{b-a}{N} f(x_k) = \frac{b-a}{N} \sum_{k=0}^{N-1} f(x_k).$$

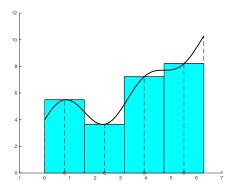


Figure: Midpoint composite rule and approximation of  $\int_0^{2\pi} 3 + \sin(2x) + \cos(x) + x \, dx$  (the formula computes the area in cyan).

# Theorem (Error of midpoint composite rule)

If [a, b] is subdivided in N equispaced intervals of length  $h = \frac{b-a}{N}$ , then

$$E_0^{(c)}(f) := I(f) - S_0^{(c)}(f, a, b, N) = \frac{(b-a)}{24} h^2 f^{(2)}(\xi^*), \ \xi^* \in (a, b)$$

# Remark (Degree of exactness)

From the formula above, it is immediate to get that ADE is exactly equal to 2.

# Remark (Comparison with the midpoint rule)

The midpoint rule had an error

$$E_0(f) := I(f) - S_0(f) = \frac{(b-a)^3}{24} f^{(2)}(\xi), \ \xi \in (a,b),$$

while for N > 1

$$\frac{(b-a)}{24}h^2 = \frac{(b-a)}{24}\left(\frac{b-a}{N}\right)^2 = \frac{(b-a)^3}{24N^2} < \frac{(b-a)^3}{24}.$$

Consequently, one may think that if  $f^2$  does not vary much, the composite rule tend to provide smaller errors (notice that in general  $\xi^* \neq \xi$ ).

### Purpose. (How it is obtained)

To give some insight, suppose that [a,b] is subdivided N=4 equispaced subintervals  $[t_k,t_{k+1}]$ ,  $K=0,\ldots,N-1=3$  con  $t_j=a+jh$ ,  $j=0,\ldots,N=4$ , h=(b-a)/N=(b-a)/4.

Let  $S_1(f, \alpha, \beta)$  the application of the trapezoidal rule relatively to f and to the interval  $[\alpha, \beta]$ ,

- $S_1(f, t_0, t_1) = \frac{h}{2}(f(t_0) + f(t_1)),$
- $S_1(f, t_1, t_2) = \frac{h}{2}(f(t_1) + f(t_2)),$
- $S_1(f, t_3, t_4) = \frac{h}{2}(f(t_3) + f(t_4)),$

thus being N=4

$$S_{1}^{(c)}(f, a, b, 4) = \frac{h}{2}(f(t_{0}) + f(t_{1}) + f(t_{1}) + f(t_{2}) + f(t_{2}) + f(t_{3}) + f(t_{3}) + f(t_{4}))$$

$$= \frac{h}{2}(f(t_{0}) + 2f(t_{1}) + 2f(t_{2}) + 2f(t_{3}) + f(t_{4}))$$

$$= \frac{b - a}{N} \left(\frac{1}{2}f(t_{0}) + f(t_{1}) + f(t_{2}) + f(t_{3}) + \frac{1}{2}f(t_{4})\right)$$

# Definition (Trapezoidal composite rule)

Let  $x_k = a + kh$ , k = 0, ..., N, h = (b - a)/N, the trapezoidal composite rule is defined as

$$S_1^{(c)}(f,a,b,N) := \frac{b-a}{N} \left[ \frac{f(x_0)}{2} + f(x_1) + \ldots + f(x_{N-1}) + \frac{f(x_N)}{2} \right],$$

In the previous assumptions,

$$E_1^{(c)}(f) := I(f) - S_1^{(c)}(f, a, b, N) = \frac{-(b-a)}{12}h^2f^{(2)}(\xi), \ h = \frac{(b-a)}{N} \ \xi \in (a, b).$$

### Remark (Grado di exactness)

Similarly to the basic rule, the degree of precision is exactly 1 since

$$|E_1^{(c)}(f)| := |I(f) - S_1^{(c)}(f, a, b, N)| = \frac{(b-a)}{12}h^2|f^{(2)}(\xi)|, \ h = \frac{(b-a)}{N},$$

### Remark (Comparison with the rule)

With regards to the rule, we had

$$|E_1(f)| := |I(f) - S_1(f)| = \frac{(b-a)^3}{12} |f^{(2)}(\xi)|, \ \xi \in (a,b).$$

but here, being N > 1

$$\frac{(b-a)}{12}h^2 = \frac{(b-a)}{12}\left(\frac{(b-a)}{N}\right)^2 = \frac{(b-a)^3}{12N^2} < \frac{(b-a)^3}{12},$$

and as in the case of the midpoint composite rule, we expect an inferior error increasing N if  $f^2$  does not vary much.

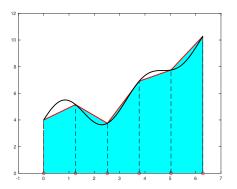


Figure: Trapezoidal composite rule for approximating  $\int_0^{2\pi} 3 + \sin(2x) + \cos(x) + x \, dx$  (it computes the area in cyan, that is the area defines by the piecewise interpolant in red).

The trapezoidal composite rule has many interesting features., that are carefully described in [?]. In particular we can consider a note on a work by Poisson.

It appears to have been Poisson, in the 1820s, who first identified this effect [139]. The example Poisson chose has remained a favorite ever since: the perimeter of an ellipse, which he took to have axis lengths  $1/\pi$  and  $0.6/\pi$ , giving the integral

(1.1) 
$$I = \frac{1}{2\pi} \int_{0}^{2\pi} \sqrt{1 - 0.36 \sin^2 \theta} \, d\theta.$$

Poisson used this now-standard notation for definite integrals, but apparently it was not yet standard in the 1820s, for he comments that

pour indiquer [les limites de l'intégrale] en même temps que l'intégrale, nous emploierons la notation très-commode que M. Fourrier a proposée.  $^1$ 

Perhaps in 1826 the spelling of Fourier's name wasn't yet standardized either! The exact solution of (1.1) is

(1.2) 
$$I = \frac{2}{\pi}E(0.36) = 0.90277992777219...,$$

where E is the complete elliptic integral of the second kind. As trapezoidal rule approximations we can take

$$I_N = \frac{1}{N} \sum_{k=1}^{N} \sqrt{1 - 0.36 \sin^2(2\pi k/N)}$$

for any positive integer N, or, equivalently, if N is divisible by 4, exploiting the four-fold symmetry as Poisson did,

$$I_N = \frac{4}{N} \sum_{k=0}^{N/4} \sqrt{1 - 0.36 \sin^2(2\pi k/N)}.$$

#### Eulero-Maclaurin formula

Consider the integrand

$$\frac{1}{2\pi}\sqrt{1-0.36\sin^2\theta}$$

and verify it is periodic with its derivatives in  $[0, 2\pi]$ . Both the geometry (meaning of the integral) and Maple confirm this.

```
>> syms f(x)
>> f(x)=(1/(2*pi))*sqrt(1-0.36*(sin(x))^2);
>> g=diff(f,x,1); g(2*pi)-g(0)
ans = 0
>> g=diff(f,x,2); g(2*pi)-g(0)
ans = 0
>> g=diff(f,x,3); g(2*pi)-g(0)
ans = 0
>> g=diff(f,x,4); g(2*pi)-g(0)
ans = 0
\Rightarrow g=diff(f,x,25); g(2*pi)-g(0)
ans = 0
\Rightarrow g=diff(f,x,30); g(2*pi)-g(0)
ans = 0
```

### Euler-Maclaurin formula

Let  $h_N$  be the length of the generic subinterval of the equispaced subdivision of [a,b].

#### Theorem (Euler-Mac Laurin formula, 1735)

If  $f \in C^{2M+2}([a,b])$  then

$$\int_{a}^{b} f(x)dx = S_{1}^{(c)}(f,N) + \sum_{k=1}^{M} \frac{B_{2k}}{(2k)!} h_{N}^{2k} \left( f^{(2k-1)}(b) - f^{(2k-1)}(a) \right)$$
$$- \frac{B_{2M+2}}{(2M+2)!} h_{N}^{(2M+2)}(b-a) f^{(2M+2)}(\xi), \ \xi \in (a,b)$$

where  $B_k$  are the Bernoulli numbers (Bernoulli, 1713).

If 
$$f \in C^{2M+2}([a,b])$$
 e  $f^{(2k-1)}(b) = f^{(2k-1)}(a)$ , for  $k = 1, \dots, M$ 

$$\int_a^b f(x)dx - S_1^{(c)}(f,N) = -\frac{B_{2M+2}}{(2M+2)!}h_N^{(2M+2)}(b-a)f^{(2M+2)}(\xi),$$

where  $\xi \in (a,b)$  and from  $h_N = (b-a)/N$ , we get  $\mathcal{E}_1^{(c)}(f) \approx \frac{C}{N^{2M+2}}$ .

### Euler-Maclaurin formula (Bernoulli numbers)

Bernoulli numbers might have been the first quantities computes numerically by a code on a machine, the so called Analytical Engine (1842), that is considered as the first modern calculator.

There is a controversy if the programmer was Babbage, the designer of the machine or Ada Lovelace, daughter of Lord Byron.



Figure: A component of the Analytical Engine.

#### Euler-Maclaurin formula

From Euler-Mac Laurin formula, in the case of  $f(\theta) := \frac{1}{2\pi} \sqrt{1 - 0.36 \sin^2 \theta}$  we have that

$$|E_1^{(c)}(f)| := |\int_a^b f(x)dx - S_1^{(c)}(f, N)|$$

is more rapid than  $N^{-M}$  for any M (here N is the number of subintervals).

Actually it is of *geometric* type, that is  $|E_1^{(c)}(f)| \approx \alpha \gamma^{-N}$ , for suitable  $\alpha$ ,  $\gamma$  (cf. [?], p.387). he

N	$ E_1^{(c)}(f) $	N	$ E_1^{(c)}(f) $
2	9.7 <i>e</i> – 02	32	0
4	2.8 <i>e</i> – 03	64	0
8	1.1e — 05	128	0
16	5.4e — 10	256	0
32	1.1 <i>e</i> — 16	512	0

Table: Error of Trapezoidal composite rule on Poisson example, subdividing [a,b] in N equispaced intervals

# Trapezoidal composite rule: applications

Numerical integration of periodic functions is an important subject due to its applications.

It is a fundamental ingredient of FFT algorithm that requires the evaluations of these quantities for specific integrands.

The Fast Fourier Transform is used in

- elaboration of digital signals (fundamental for the mp3 compression),
- solution of PDEs;
- algorithms for multiplication of integers of large magnitude.

This algorithm was discovered by Cooley-Tukey in 1965 (but some sources say it was known is some form to Gauss!).

#### Remark

In IEEE Guest Editors' Introduction: The Top 10 Algorithms. it is written:

The FFT is perhaps the most ubiquitous algorithm in use today to analyze and manipulate digital or discrete data.

#### Purpose. (Composite Cavalieri-Simpson rule)

As illustration, let us subdivide [a, b] in N = 4 equispaced intervals  $[t_k, t_{k+1}]$ ,  $k = 0, \dots, N - 1 = 3$  with  $t_j = a + jh$ ,  $j = 0, \dots, N = 4$ , h = (b - a)/N.

Defining with  $S_2(f, t_k, t_{k+1})$  the application of Cavalieri-Simpson rule relatively to f and to the interval  $[t_k, t_{k+1}]$ , letting  $c_k = \frac{t_k + t_{k+1}}{2} = a + \frac{2k+1}{2} \cdot \frac{b-a}{N}$  be the midpoint of  $[t_k, t_{k+1}]$ ,

$$S_2(f,t_0,t_1) = \frac{h}{6}(f(t_0) + 4 \cdot f(c_0) + f(t_1)),$$

$$S_2(f, t_1, t_2) = \frac{h}{6}(f(t_1) + 4 \cdot f(c_1) + f(t_2)),$$

$$S_2(f, t_2, t_3) = \frac{h}{6}(f(t_2) + 4 \cdot f(c_2) + f(t_3)),$$

$$S_2(f, t_3, t_4) = \frac{h}{6}(f(t_3) + 4 \cdot f(c_3) + f(t_4)),$$

we obtain from N=4

$$S_{2}^{(c)}(f, a, b, 4) = \frac{h}{6}(f(t_{0}) + 4 \cdot f(c_{0}) + f(t_{1})) + \frac{h}{6}(f(t_{1}) + 4 \cdot f(c_{1}) + f(t_{2}))$$

$$+ \frac{h}{6}(f(t_{2}) + 4 \cdot f(c_{2}) + f(t_{3})) + \frac{h}{6}(f(t_{3}) + 4 \cdot f(c_{3}) + f(t_{4})) = \dots$$

$$= \frac{h}{6}f(t_{0}) + \frac{2h}{6}(f(t_{1}) + f(t_{2}) + f(t_{3})) + \frac{h}{6}f(t_{4})$$

$$+ \frac{4h}{6}(f(c_{0}) + f(c_{1}) + f(c_{2}) + f(c_{3})).$$
 (6)

From

$$S_{2}^{(c)}(f, a, b, 4) = \frac{h}{6}f(t_{0}) + \frac{2h}{6}(f(t_{1}) + f(t_{2}) + f(t_{3})) + \frac{h}{6}f(t_{4}) + \frac{4h}{6}(f(c_{0}) + f(c_{1}) + f(c_{2}) + f(c_{3})).$$
(7)

setting  $t_0 = x_0$ ,  $c_0 = x_1$ ,  $t_1 = x_2$ ,  $c_1 = x_3$ ,  $t_2 = x_4$ ,  $c_2 = x_5$ ,  $t_3 = x_6$ ,  $c_3 = x_7$ ,  $t_4 = x_8$ , we get for N = 4 (i.e. the number of subdivisions)

$$S_2^{(c)}(f,a,b,4) = \frac{h}{6} \left( f(x_0) + 2 \sum_{r=1}^{N-1} f(x_{2r}) + 4 \sum_{s=0}^{N-1} f(x_{2s+1}) + f(x_{2N}) \right)$$
(8)

This ideas can be easily generalized to any N.

Figure: Relation between  $t_k$ ,  $c_k$  e  $x_j$ .

### Definition (Cavalieri-Simpson composite rule)

Set  $x_k = a + kh/2$ , k = 0, ..., 2N, h = (b - a)/N, Cavalieri-Simpson composite rule is defined as

$$S_2^{(c)}(f,a,b,N) = \frac{h}{6} \left[ f(x_0) + 2 \sum_{r=1}^{N-1} f(x_{2r}) + 4 \sum_{s=0}^{N-1} f(x_{2s+1}) + f(x_{2N}) \right]$$
(9)

#### Theorem (Error of Cavalieri-Simpson composite rule)

In the assumptions of subvisions via equispaced intervals of length h, the integration error is

$$E_2^{(c)}(f) := I(f) - S_2^{(c)}(f, a, b, N) = \frac{-(b-a)}{180} \left(\frac{h}{2}\right)^4 f^{(4)}(\xi), \quad \xi \in (a, b)$$

#### Remark (Degree of exactness of Cavalieri-Simpson composite rule)

The degree of exactness is exactly 3, as Cavalieri-Simpson rule, but if N > 1 the length h is inferior and consequently an inferior absolute integration error is expected.

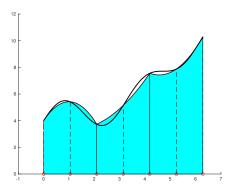


Figure: Cavalieri-Simpson composite rule for the computation of  $\int_0^{2\pi} 3 + \sin(2x) + \cos(x) + x \, dx$  (the rule determines the area in cyan).

In this section we analyse some examples in which we apply composite rules to integrate some test integrands in  $f \in C([a,b])$ .

## Example (1)

Approximate the definite integral

$$I = \int_0^{\pi} \exp(x) \cos(x) dx = -(\exp(\pi) + 1)/2.$$

by means of composite rules  $S_k^{(c)}(f, 0, \pi, N)$ , N = 1, 2, 4, ..., 512, k = 0, 1, 2.

### Remark

Note that the integrand belongs to  $C^{\infty}([0,2\pi])$  (actually it is entire).

# Some numerical comparisons: example 1

N	$ E_0^{(c)}(f) $	$ E_1^{(c)}(f) $	$ E_2^{(c)}(f) $	$\#_N^{R}$	$\#_N^T$	$\#_N^{CS}$
1	1.2 <i>e</i> + 01	2.3e + 01	4.8 <i>e</i> – 01	1	2	3
2	2.8 <i>e</i> + 00	5.3e + 00	8.5e - 02	2	3	5
4	6.4 <i>e</i> – 01	1.3e + 00	6.1 <i>e</i> - 03	l .	_	9
8	1.6 <i>e</i> – 01	3.1e — 01	3.9e - 04	8	9	17
16	3.9 <i>e</i> – 02	7.8 <i>e</i> – 02	2.5e - 05	16	17	33
32	9.7 <i>e</i> – 03	1.9 <i>e</i> – 02	1.6 <i>e</i> – 06	32	33	65
64	2.4 <i>e</i> – 03	4.8e - 03	9.7e - 08	64	65	129
128	6.1 <i>e</i> – 04	1.2 <i>e</i> – 03	6.1 <i>e</i> – 09	128	129	257
256	1.5 <i>e</i> — 04	3.0e - 04	3.8e - 10	256	257	513
512	3.8 <i>e</i> — 05	7.6 <i>e</i> – 05	2.4 <i>e</i> – 11	512	513	1025

Table: Comparison of midpoint, trapezoidal and Cavalieri-Simpson composite rule, for N equispaced intervals relatively to the computation of  $I = \int_0^\pi f(x) dx$  con  $f(x) = \exp(x) \cos(x) dx$ , describing the absolute errors  $|E_0^{(c)}(f)| = |I(f, a, b) - S_0^{(c)}(f, a, b, N), |E_1^{(c)}(f)| = |I(f, a, b) - S_1^{(c)}(f, a, b, N)|, |E_2^{(c)}(f)| = |I(f, a, b) - S_2^{(c)}(f, a, b, N)|, for each formula and the respective number of nodes <math>\#_N^R$ ,  $\#_N^T$ ,  $\#_N^T$ .

## Some numerical comparisons: example 1 (optional)

## Remark (optional)

In the second table we show the ratio between two successive errors for each formula. The value  $(E_k^{(c)}(f))_N$ , k=0,1,2, is the absolute integration error by  $S_k$ , for computing  $\int_a^b f(x) dx$ , over N subdivisions, while

$$(r_k^{(c)}(f))_N = \frac{(E_k^{(c)}(f))_N}{(E_k^{(c)}(f))_{2N}}$$

is the ratio for k = 0,1,2 (in order, midpoint, trapezoidal and Cavalieri-Simpson composite rule).

# Some numerical comparisons: example 1 (optional)

N	$(r_0^{(c)}(f))_N$	$(r_1^{(c)}(f))_N$	$(r_2^{(c)}(f))_N$
1	4.33	4.27	5.59
2	4.34	4.20	13.92
4	4.10	4.06	15.54
8	4.03	4.02	15.89
16	4.01	4.00	15.97
32	4.00	4.00	15.99
64	4.00	4.00	16.00
128	4.00	4.00	16.00
256	4.00	4.00	16.00

Table: Ratios relatively to  $I = \int_0^{\pi} f(x)dx$  with  $f(x) = \exp(x)\cos(x)dx$ , showing the ratios between two successive absolute errors of the formulas.

### Example (2)

Approximate the definite integral

$$I = \int_{-5}^{5} \frac{1}{1+x^2} dx \approx 2.7468015338900322319659608$$

by composite rules  $S_k^{(c)}(f, -5, 5, N)$ , N = 1, 2, 4, ..., 1024, k = 0, 1, 2.

### Remark

The integrand belongs to  $C^{\infty}([-5,5])$ . Thus we can apply the error theorems for all the composite rules.

# Some numerical comparisons: example 2

N	$ E_0^{(c)}(f) $	$ E_1^{(c)}(f) $	$ E_2^{(c)}(f) $	$\#_N^{R}$	$\#_N^T$	$\#_N^{CS}$
1	7.3e + 00	2.4e + 00	4.0e + 00	1	2	3
2	1.4e + 00	2.4e + 00	9.6e - 02	2	3	5
4	4.6 <i>e</i> – 01	5.4e - 01	1.3 <i>e</i> – 01	4	5	9
8	3.9 <i>e</i> – 02	3.8e - 02	1.3 <i>e</i> – 02	8	9	17
16	2.1 <i>e</i> – 04	6.9e - 04	9.1 <i>e</i> – 05	16	17	33
32	1.2 <i>e</i> – 04	2.4e - 04	4.5e - 08	32	33	65
64	3.0 <i>e</i> – 05	6.0e - 05	2.6e - 09	64	65	129
128	7.5 <i>e</i> – 06	1.5e — 05	1.6e — 10	128	129	257
256	1.9 <i>e</i> – 06	3.8e - 06	1.0 <i>e</i> – 11	256	257	513
512	4.7 <i>e</i> – 07	9.4e - 07	6.4e - 13	512	513	1025
1024	1.2e — 07	2.4 <i>e</i> – 07	4.0e — 14	1024	1025	2049

Table: Comparison of midpoint, trapezoidal and Cavalieri-Simpson composite rule, for N equispaced intervals relatively to the computation of  $I = \int_{-5}^{5} f(x) dx$  con  $f(x) = 1/(1+x^2)$ , describing the absolute errors  $|E_0^{(c)}(f)| = |I(f, a, b) - S_0^{(c)}(f, a, b, N)$ ,  $|E_1^{(c)}(f)| = |I(f, a, b) - S_2^{(c)}(f, a, b, N)|$ , for each formula and the respective number of nodes  $\#_N^H$ ,  $\#_N^H$ .

# Some numerical comparisons: example 3 (optional)

### Example (3)

Approximate the definite integral

$$I = \int_0^1 x^3 \sqrt{x} dx = 2/9.$$

by composite rules  $S_k^{(c)}(f, 0, 1, N)$ , N = 1, 2, 4, ..., 1024, k = 0, 1, 2.

### Remark

The integrand belongs to  $C^3([0,1])$ . Thus we can take into account all the error formulas but that of composite Cavalieri-Simpson rule that requires  $f \in C^4([0,1])$ 

# Some numerical comparisons: example 3

N	$ E_0^{(c)}(f) $	$ E_1^{(c)}(f) $	$ E_2^{(c)}(f) $	$\#_N^{R}$	$\#_N^T$	$\#_N^{CS}$
1	1.3 <i>e</i> – 01	2.8 <i>e</i> – 01	3.4 <i>e</i> – 03	1	2	3
2	3.6 <i>e</i> – 02	7.2e - 02	2.3e - 04	2	3	5
4	9.1 <i>e</i> – 03	1.8 <i>e</i> – 02	1.5 <i>e</i> – 05	4	5	9
8	2.3 <i>e</i> – 03	4.6e - 03	1.0 <i>e</i> – 06	8	9	17
16	5.7e — 04	1.1e — 03	6.5e - 08	16	17	33
32	1.4 <i>e</i> – 04	2.8e - 04	4.1e - 09	32	33	65
64	3.6 <i>e</i> – 05	7.1 <i>e</i> – 05	2.6 <i>e</i> – 10	64	65	129
128	8.9 <i>e</i> – 06	1.8 <i>e</i> – 05	1.7 <i>e</i> — 11	128	129	257
256	2.2 <i>e</i> – 06	4.5e - 06	1.0 <i>e</i> – 12	256	257	513
512	5.6 <i>e</i> – 07	1.1 <i>e</i> – 06	6.6 <i>e</i> – 14	512	513	1025
1024	1.4e — 07	2.8 <i>e</i> – 07	4.1 <i>e</i> – 15	1024	1025	2049

Table: Comparison of midpoint, trapezoidal and Cavalieri-Simpson composite rule, for N equispaced intervals relatively to the computation of  $I=\int_0^1 f(x)dx$  con  $f(x)=x^3\sqrt{x}dx$ , describing the absolute errors  $|E_0^{(c)}(f)|=|I(f,a,b)-S_0^{(c)}(f,a,b,N),$   $|E_1^{(c)}(f)|=|I(f,a,b)-S_2^{(c)}(f,a,b,N)|$ , for each formula and the respective number of nodes  $\#_N^R$ ,  $\#_N^T$ ,  $\#_N^{CS}$ .

# Remark (optional)

In the second table we show the ratio between two successive errors for each formula. The value  $(E_k^{(c)}(f))_N$ , k=0,1,2, is the absolute integration error by  $S_k$ , for computing  $\int_a^b f(x) dx$ , over N subdvisions, while

$$(r_k^{(c)}(f))_N = \frac{(E_k^{(c)}(f))_N}{(E_k^{(c)}(f))_{2N}}$$

is the ratio for k = 0,1,2 (in order, midpoint, trapezoidal and Cavalieri-Simpson composite rule).

From the tables we see that the ratio for

- composite midpoint and trapezoidal rule is approximatively 4,
- composite Cavalieri-Simpson rule is approximatively 16, and thus the errors are of the form  $C^*h^2$  and  $C^*h^4$ .