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OPTIMAL NUMERICAL INTEGRATION BY GAUSS-LEGENDRE QUADRATURES

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Abstract

We will consider the problem of numerical quadrature of a definite integral in cases where the integrand is not explicitly known, ie it is given in the form of tabular data or as a points (x_i, y_i), or when the function can not be integrated with elementary algebraic transformations. We will briefly describe the Newton-Cotes integration formulas and their corresponding error estimates. Furthermore, we will provide a general form of Gauss quadrature formulas in which weight functions are orthogonal polynomials. In this paper, we will consider numerically integrating Gauss-Legedre's formulas, that is, when the weight function is in the Legendre polynomial class. We will show two ways to generate Legendre polynomials and some of them will be graphically presented. Using the *Mathematica* program package through specific examples for numerical computation of the integral, when comparing the results with classical Newton-Cotes formulas, it turns out that Gauss-Legedre's quadratures give apparent better results in evaluating the error of the method, as well as with a reduced number of steps in executing the algorithm to achieve the required accuracy.

Keywords: *Numerical integration methods, Newton-Cotes formulas, orthogonal polynomials, Gauss-Legendre quadrature, error estimates.*

Introduction

If the function $f : I \to \mathbb{R}$ is continuous and $F : I \to \mathbb{R}$ is any primitive function of the function f on interval I, then for each segment $[a,b] \subseteq I$ it is valid,

$$\int_a^b f(x)dx = F(b) - F(a).$$

The given formula is the Newton-Leibniz formula for computing the Riemann integral of the function f on the segment $[a,b]$.

In the various applications of a definite integral, it has not been possible to calculate integral with this formula. The reason is that a large number of functions can not determine the primitive function in an elementary way or is very difficult to find. Furthermore, often in applications, function f is given in the form of tabular data or as a solution of the differential equation. To calculate the integral of such functions, there is a need to introduce numerical methods by which we approximate the values of these integrals.

Below we provide examples of several functions whose integral can be calculated solely by numerical methods.

Example 0.1. In probability theory, integrals are often encountered, which are not be resolved explicitly, but some numerical methods are needed. One such example is the distribution function of the standard normal distribution, which is accounted for as:

$$G(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{1}{2}t^2} dt, \quad (x \in \mathbb{R}).$$

Example 0.2. Fresnel integrals, designated as functions $I_S(x)$ and $I_C(x)$, and their application in physics and technique: $I_S(x) = \int_0^x \sin\left(\frac{\pi}{2}t^2\right) dt, \ (x \in \mathbb{R}^+)$

$$I_C(x) = \int_0^x \cos\left(\frac{\pi}{2}t^2\right) dt, \quad (x \in \mathbb{R}^+).$$

Therefore, when the integral value can not be exactly computed by standard procedures, we use numeric methods.

Numerical methods

The basic idea of all methods is to compute the approximation of the integral

$$\int_a^b f(x)dx$$

using the function values in points x_i, where $x_i \in [a,b]$ for $i = 1,2,...,n$.

One of the obvious ways of solving this problem is to approximate the function f with a simple, easy-to-integrate function, most commonly by interpolation polynomial. The symbol for the approximation of the integral will be I^*, and in general we can write it as

$$I^* = \sum_{i=1}^{n} \omega_i f(x_i).$$

Such a record is called a numeric quadrature formula or a numerical integration formula. The next important term that appears is

the error of approximation. We will mark it with

$$E = \Delta I^* = \left| I - I^* \right|.$$

For each method, the error rating will be defined. Here will be briefly explained the trapezoidal rule and Newton-Cotese's formula, so that we can compare them in this paper with Gaussian quadratic formulas.

Generalized trapezoidal formula

If the continuous function $f : I \to \mathbb{R}$ is replaced by the first-degree polynomial in the interpolation points $(a, f(a)), (b, f(b))$, then the approximation is:

$$I^* = \int_a^b p_1(x)dx = \frac{b-a}{2}[f(b) - f(a)]$$
(P)

For error estimation can be taken

$$E = \Delta I^* = \left|I - I^*\right| \le \max_{a \le x \le b}\left|f''(x)\right| \cdot \frac{(b-a)^3}{12n^2}.$$

In the equidistant division of the interval $[a,b]$, the formula (P) is applied to each small segment of the $[x_{i-1}, x_i]$ and an approximation of the generalized trapezoidal formula is obtained

$$I^* = \frac{b-a}{2n}\left[y_0 + 2(y_1 + ... + y_{n-1}) + y_n\right].$$

Generalized Simpson formula

If in the segment $[a,b]$ except the end points a and b, we also take the middle point $\frac{a+b}{2}$, then the function f at the interval I is replaced by the polynomial of the second degree $p_2(x)$ passing through these points. In this case, the approximation of the integral is

$$I^* = \int_a^b p_2(x)dx = \frac{b-a}{6}\left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right]$$
(S)

Error estimation is

$$E = \Delta I^* = \left|I - I^*\right| \le \max_{a \le x \le b}\left|f^{(4)}(x)\right| \cdot \frac{(b-a)^5}{180n^4}.$$

When the formula (S) is applied to each $[x_{i-1}, x_i]$ division, the approximation of the generalized Simpson formula is obtained:

$$I^* = \frac{b-a}{3n}\left[y_0 + 2(y_2 + y_4 + ... + y_{n-2}) + 4(y_1 + y_3 + ... + y_{n-1}) + y_n\right].$$

Gaussian quadrature formulas

In previous methods, we used the given n-nodes to accurately calculate the integral value using the interpolation polynomial of degree at most n. We wonder if we can construct formulas by which we calculate integrals of polynomial whose degree is greater than the interpolation polynomial. This property will have Gaussian quadrature.

Gaussian integration formulas are generally of a form

$$\int_a^b \omega(x)f(x)dx = \sum_{i=1}^{n}\omega_i(x)f(x_i)$$
(*)

where $\omega(x)$ is a weighting function, positive or at least non-negative and integrable on $[a,b]$, $\omega_i(x)$ are weight coefficients, and x_i integration nodes. In this paper we will use a special case, when $\omega(x) \equiv 1$. Depending on the choice of weight function, the Gaussian formula assumes a different form and name.

weight function $\omega(x)$	interval	formula
1	$[-1,1]$	Gauss-Legendre
$\frac{1}{\sqrt{1-x^2}}$	$[-1,1]$	Gauss-Chebyshev
e^{-x}	$[0,+\infty)$	Gauss-Laguerre
e^{-x^2}	$(-\infty,+\infty)$	Gauss-Hermit

Definition. The degree of accuracy of the quadrature formula is the largest number of $m \in \mathbb{N}$ such that $E(x^k) = 0$, for each $k = 0,1,...,m$, but is $E(x^k + 1) \neq 0$.

The value of the integral $I = \int_a^b f(x)dx$ is approximated by a quadrature formula which is generally in the form

$$I^* = \sum_{i=1}^{n} \omega_i(x) f(x_i).$$

We want this formula to be the degree of precision *m*, that is, it is valid

$$\int_a^b x^k dx - \sum_{i=1}^{n} \omega_i x_i^k = 0, \quad \text{for each } k = 0,1,...,m.$$

Gauss-Legendre's quadrature formula

We will use a family that consists of Legendre's polynomials, defined in the $[-1,1]$ segment. As the process does not generally depend on the area of integration, we will use substitution

$$x = \frac{b-a}{2} t + \frac{b+a}{2}$$

From which it follows

$$\int_a^b f(x)dx = \frac{b-a}{2} \int_{-1}^{1} f\left(\frac{b-a}{2} t + \frac{b+a}{2}\right) dt$$

Let us denote the

$$\phi(t) = f\left(\frac{b-a}{2} t + \frac{b+a}{2}\right),$$

using the formula (*), we get an approximate quadratic formula

$$I^* = \frac{b-a}{2} \sum_{i=1}^{n} \omega_i \phi(t_i).$$

Remark. Coefficients of ω_i and t_i nodes are unknown to us. Nodes will be counted as the null Legendre polynomials.

For two functions $f, g : [a,b] \to \mathbb{R}$, we say that they are mutually orthogonal if they are valid

$$f \cdot g = \int_a^b f(x) \cdot g(x) dx = 0.$$

One of the methods of constructing Legendre polynomials is the Gram-Schmidt method of orthogonalization of the canonical base of $\{1, x, x^2, ...\}$.

So obtained polynomials are

$P_0(x) = 1$

$$P_1(x) = x - \frac{(x, P_0)}{(P_0, P_0)} \cdot P_0(x) = x$$

$$P_2(x) = x^2 - \frac{(x^2, P_0)}{(P_0, P_0)} \cdot P_0(x) - \frac{(x^2, P_1)}{(P_1, P_1)} \cdot P_1(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_3(x) = x^3 - \frac{(x^3, P_0)}{(P_0, P_0)} \cdot P_0(x) - \frac{(x^3, P_1)}{(P_1, P_1)} \cdot P_1(x) - \frac{(x^3, P_2)}{(P_2, P_2)} \cdot P_2(x) = ... = \frac{1}{2}(5x^3 - 3x)$$

$$P_4(x) = x^4 - \frac{(x^4, P_0)}{(P_0, P_0)} \cdot P_0(x) - \frac{(x^4, P_1)}{(P_1, P_1)} \cdot P_1(x) - \frac{(x^4, P_2)}{(P_2, P_2)} \cdot P_2(x) - \frac{(x^4, P_3)}{(P_3, P_3)} \cdot P_3(x) = ... = \frac{1}{8}(35x^4 - 30x^2 + 3)$$

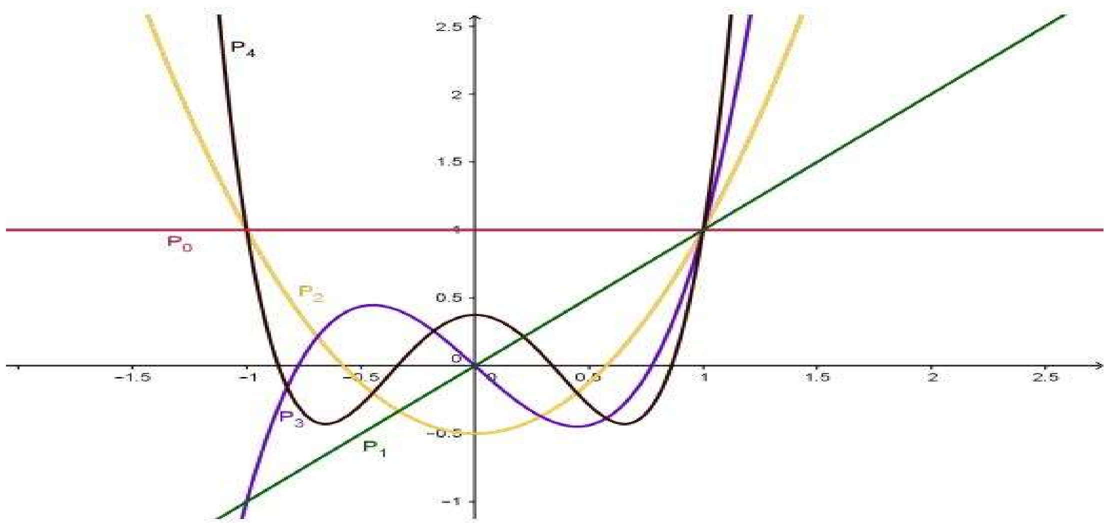

Figure 1. Graphic view of the first five Legendre polynomials

Nodes integration count as zeros of polynomials $P_0, P_1, P_2, P_3, P_4, ...$

Example. Calculate integration nodes for $n = 3$. Searching for zeros of Legendre polynomial P_3 of the third degree.

$$P_3(x) = 0$$

$$x^3 - \frac{3x}{5} = 0$$

Zeros, or nodes integration are:

$$x_1 = -\sqrt{\frac{3}{5}}, \quad x_2 = 0, \quad x_3 = \sqrt{\frac{3}{5}}.$$

It still remains to calculate the weighted coefficients ω_i.

Let $x_i \in [-1, 1]$ and let

$$p_{n-1,i} = \frac{(x-x_1)...(x-x_{i-1})(x-x_{i+1})...(x-x_n)}{(x_i-x_1)...(x_i-x_{i-1})(x_i-x_{i+1})...(x_i-x_n)}$$

The polynomials $p_{n-1,i}$ are Lagrange's interpolation polynomials of degree $(n-1)$, hence the Gaussian quadrature formula calculates exactly their integrals.

$$\int_{-1}^{1} p_{n-1,i}\, dx = \sum_{i=1}^{n} \omega_i p_{n-1,i}$$

Since the

$$p_{n-1,i}(x_j) = \delta_{i,j}$$

From which it follows

$$\int_{-1}^{1} p_{n-1,i}\, dx = \omega_i .$$

In the example above, for $n=3$, we compute nodes, now we calculate the weight coefficients according to the formula

$$\omega_1 = \int_{-1}^{1} p_{2,1}\, dx = \int_{-1}^{1} \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} dx = \frac{5}{6}\int_{-1}^{1}\left(x^2 - \sqrt{\frac{3}{5}}x \right) dx = ... = \frac{5}{9}$$

$$\omega_2 = \int_{-1}^{1} \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} dx = ... = \frac{8}{9}$$

$$\omega_3 = \int_{-1}^{1} \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} dx = ... = \frac{5}{9}$$

Note. The integration nodes are located in symmetrical points with respect to origin, and the coefficients of symmetric nodes are equal.

Lema 1. Each Legendre polynomial of degree n is orthogonal to polynomial degree $< n$.
Lema 2. Let the weight coefficients be given by the formula

$$\omega_i = \int_{-1}^{1} p_{n-1,i}\, dx$$

Then the quadrature formulas exact for polynomials of degree $n-1$.

Theorem 1. Let the coefficients of the quadrature formula be calculated by Lema 2 and let the nodes of the formula be a zeros of the Legendre polynomial $P_n(x)$. Then this formula is exact for the polynomial of degree $2n-1$.
Theorem 2. Let $f \in C^{2n}([a,b])$ be the given function. Then there is a point $c \in [a,b]$ such that for the Gaus-Legendre error estimation method integration is valid

$$E_n = \frac{(b-a)^{2n+1}(n!)^4}{(2n+1)((2n)!)^3} f^{(2n)}(c).$$

In the following table are listed the calculated values of integration nodes and weights for several cases.

$n=2$	
$x_1=-1/\sqrt{3}$	$\omega_1=1$
$x_2=1/\sqrt{3}$	$\omega_2=1$
$n=3$	
$x_1=-\sqrt{3}/\sqrt{5}$	$\omega_1=5/9$
$x_2=0$	$\omega_2=8/9$
$x_3=\sqrt{3}/\sqrt{5}$	$\omega_3=5/9$
$n=4$	
$x_1=-0.861136$	$\omega_1=0.347855$
$x_2=-0.339981$	$\omega_2=0.652145$
$x_3=0.339981$	$\omega_3=0.652145$
$x_4=0.861136$	$\omega_4=0.347855$
$n=5$	
$x_1=-0.90618$	$\omega_1=0.236927$
$x_2=-0.538469$	$\omega_2=0.478629$
$x_3=0$	$\omega_3=0.568889$
$x_4=0.538469$	$\omega_4=0.478629$
$x_5=0.90618$	$\omega_5=0.236927$

Table 2. Gauss-Legendre quadrature formula

Numerical experiments and results

Example 1. Calculate the integral of the function $f(x)=\sqrt{1+3x}$ on the $[0,1]$ segment using the Gaus-Legendre method at 3 integration points.

We compute

$$I=\int_0^1\sqrt{1+3x}\,dx$$

Since Gauss-Legendre's method is defined in the $[-1,1]$ segment, we make a substitution

$$x=\frac{b-a}{2}t+\frac{b+a}{2}.$$

So it is

$$I=\int_0^1\sqrt{1+3x}\,dx=\frac{1}{2}\int_{-1}^1\sqrt{\frac{5}{2}+\frac{3}{2}t}\,dt.$$

The approximation of integral I is

$$I^*=\sum_{i=1}^{3}\omega_i\sqrt{\frac{5}{2}+\frac{3}{2}x_i}\ .$$

Include the data from the table above and as a result we get $I^* = 1.55561$. The exact value of the integral is $I = \frac{14}{9} \approx 1.55556$. Error in this case is

$E_3 = |I - I^*| = |1.55556 - 1.55561| = 0.00001 = 10^{-5}$.

Also, we can calculate the error estimation based on Theorem 2:

$$E_3 = \frac{(b-a)^7 (3!)^4}{7 \cdot (6!)^3} f^{(6)}(c)$$
$$= \frac{(b-a)^7}{2016000} f^{(6)}(c).$$

Comparison of methods

Example 2. Let the default function $f(x) = xe^{2x}$ be on the $[0,4]$ segment. Applying the Newton-Leibniz formula, was obtained:

$$I = \int_0^4 xe^{2x} dx = \frac{7}{4} e^8 + \frac{1}{4} \approx 5216.92648.$$

We will use the Gauss and Newton-Cotes formula to see how many steps we can get a result with an error of less than 0.01.

n	Gauss-Legendre	Newton-Cotes
1	436.785	23847.66390
2	3477.54	8240.41143
3	4967.11	6819.20880
4	5197.54	5499.67970
5	5215.99	5386.62015
6	5216.90	5239.58047
7	5216.93	5231.31978
8	5216.93	5218.33122
9	5216.93	5217.84756
10	5216.93	5216.99337

For Gauss quadrature formulas, for $n = 4$, we have an error of 0.0037, while for Newton-Cotes formula only for $n = 6$ achieves error which is less than 0.01, i.e. 0.0043.

Example 3. Let the $f(x) = e^{-\frac{1}{2}x^2}$ function be assigned to the $[0,4]$ segment. Function f is an example of a function whose integral can not be exactly calculated. Using the error estimates for the extended trapezoidal and Simpson formula, we calculate the number of steps required to achieve accuracy of $\varepsilon = 0.001$.

Generalized trapezoidal formula: If $M_2 = \max_{a \le x \le b} |f''(x)|$, then from the formula for estimating the error of approximation

$$|E_n| \le \frac{(b-a)^3}{12n^2} M_2 < \varepsilon$$

let's calculate

$$n > (b-a)\sqrt{\frac{b-a}{12\varepsilon}M_2} = 4\cdot\sqrt{\frac{4}{12\cdot 0.001}0.25} \approx 36.51.$$

The smallest n which achieves the required accuracy is $n = 37$.

Generalized Simpson formula: If $M_4 = \max_{a\le x\le b}\left|f^{(4)}(x)\right|$, then from the formula for estimating the

error of approximation $\left|E_n\right| \le \frac{(b-a)^5}{180n^4}M_4 < \varepsilon$

we calculate

$$n > (b-a)\sqrt[4]{\frac{b-a}{180\varepsilon}M_4} = 4\cdot\sqrt[4]{\frac{4}{180\cdot 0.001}0.063} \approx 4.35.$$

The smallest n which achieves the required accuracy is $n = 5$.

Gauss-Legendre formula:

$$E_n = \frac{(b-a)^{2n+1}\left(n!\right)^4}{(2n+1)\left((2n)!\right)^3}f^{(2n)}(c)$$

For $n = 3$ it follows

$$E_3 \le \frac{4^7(3!)^4}{7\cdot(6!)^3}M_6 \approx 0.00025$$

Gaus-Legendre method for $n = 3$ achieves the required accuracy.

Conclusion

With Gaus-Legendre's quadrature formula, in both cases, we achieve the required accuracy much faster. Gaussian quadrature formulas are used to achieve the maximum degree of accuracy in the approximate computation of definite integrals.

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