Chapter 6. Numerical Integration and Differentiation

Numerical Analysis 1. Winter Semester 2018-19

1 Trapezoidal, Simpson and Midpoint rules

1.1 Trapezoidal rule

1.2 Error estimation

1.3 Simpson rule

1.4 Midpoint rule rule

2 Error analysis

2.1 For Trapezoidal rule

2.2 For Simpson rule

2.3 For Midpoint rule

3 Newton-Cotes formulae

Newton-Cotes quadrature formulas for approximating $\int_a^b f(x)dx$ are obtained by approximating the function of integration $f(x)$ by interpolating polynomials. The rules are *closed* when they involve function values at the ends of the interval of integration. Otherwise, they are said to be *open*.

Some **closed Newton-Cotes rules** with error terms are as follows. Here, $a = x_0, b = x_n$, $h = (b-a)/n$, $x_i = x_0 + ih$, for $i = 0, 1, \ldots, n$, where $h = (b-a)/n$, $f_i = f(x_i)$, and $a = x_0 < \xi < x_n = b$ in the error terms.

Trapezoid Rule:

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{1}{2}h[f_0 + f_1] - \frac{1}{12}h^3 f''(\xi)$$

Simpson's $\frac{1}{3}$ Rule:

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{1}{3}h[f_0 + 4f_1 + f_2] - \frac{1}{90}h^5 f^{(4)}(\xi)$$

Simpson's $\frac{3}{8}$ Rule:

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3}{8}h[f_0 + 3f_1 + 3f_2 + f_3] - \frac{3}{80}h^5 f^{(4)}(\xi)$$

Boole's Rule:

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2}{45}h[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4] - \frac{8}{945}h^7 f^{(6)}(\xi)$$

Figure 1: [4],p.225

Some of the **open Newton-Cotes rules** are as follows:

Midpoint Rule:

$$\int_{x_0}^{x_2} f(x)\,dx = 2hf_1 + \frac{1}{24}h^3 f''(\xi)$$

Two-Point Newton-Cotes Open Rule:

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3}{2}h[f_1 + f_2] + \frac{1}{4}h^3 f''(\xi)$$

Three-Point Newton-Cotes Open Rule:

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{4}{3}h[2f_1 - f_2 + 2f_3] + \frac{28}{90}h^5 f^{(4)}(\xi)$$

Four-Point Newton-Cotes Open Rule:

$$\int_{x_0}^{x_5} f(x)\,dx = \frac{5}{24}h[11f_1 + f_2 + f_3 + 11f_4] + \frac{95}{144}h^5 f^{(4)}(\xi)$$

Figure 2: [4],p.226

Over the years, many Newton-Cotes formulas have been derived and are compiled in the handbook by Abramowitz and Stegun [1964], which is available online. Rather than using high-order Newton-Cotes rules that are derived by using a single polynomial over the entire interval, it is preferable to use a composite rule based on a low-order basic Newton-Cotes rule. There is seldom any advantage to using an open rule instead of a closed rule involving the same number of nodes. Nevertheless, open rules do have applications in integrating a function with singularities at the endpoints and in the numerical solution of ordinary differential equations as discussed in Chapter 10 and 11.

Before the widespread use of computers, the Newton-Cotes rules were the most commonly used quadrature rules, since they involved fractions that were easy to use in hand calculations. The Gaussian quadrature rules of the next section use fewer function evaluations with higher-order error terms. The fact that they involve nodes involving irrational numbers is no longer a drawback on modern computers.

4 Romberg Quadrature Formulas

5 Gaussian Quadrature Formulas

GAUSSIAN QUADRATURE THEOREM

Let q be a nontrivial polynomial of degree $n+1$ such that

$$\int_a^b x^k q(x)\,dx = 0 \qquad (0 \leqq k \leqq n)$$

Let $x_0, x_1, \ldots, x_n$ be the zeros of q. Then the formula

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i) \quad \text{where} \quad A_i = \int_a^b \ell_i(x)\,dx \tag{3}$$

with these x_i's as nodes will be exact for all polynomials of degree at most $2n+1$. Furthermore, the nodes lie in the open interval (a, b).

Figure 3: [5],p.233

With arbitrary nodes, Formula (3) will be exact for all polynomials of degree $\leqslant n$. With the Gaussian nodes, Formula (3) will be exact for all polynomials of degree $\leqslant 2n+1$.

WEIGHTED GAUSSIAN QUADRATURE THEOREM

Let q be a nonzero polynomial of degree $n+1$ such that

$$\int_a^b x^k q(x) w(x)\,dx = 0 \qquad (0 \leqq k \leqq n)$$

Let $x_0, x_1, \ldots, x_n$ be the roots of q. Then the formula

$$\int_a^b f(x) w(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

where

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \qquad \text{and} \qquad A_i = \int_a^b \ell_i(x) w(x)\,dx$$

will be exact whenever f is a polynomial of degree at most $2n+1$.

Figure 4: [5],p.235

n	Nodes x_i	Weights A_i
1	$-\sqrt{\frac{1}{3}}$	1
	$+\sqrt{\frac{1}{3}}$	1
2	$-\sqrt{\frac{3}{5}}$	$\frac{5}{9}$
	0	$\frac{8}{9}$
	$+\sqrt{\frac{3}{5}}$	$\frac{5}{9}$
3	$-\sqrt{\frac{1}{7}(3-4\sqrt{0.3})}$	$\frac{1}{2}+\frac{1}{12}\sqrt{\frac{10}{3}}$
	$-\sqrt{\frac{1}{7}(3+4\sqrt{0.3})}$	$\frac{1}{2}-\frac{1}{12}\sqrt{\frac{10}{3}}$
	$+\sqrt{\frac{1}{7}(3-4\sqrt{0.3})}$	$\frac{1}{2}+\frac{1}{12}\sqrt{\frac{10}{3}}$
	$+\sqrt{\frac{1}{7}(3+4\sqrt{0.3})}$	$\frac{1}{2}-\frac{1}{12}\sqrt{\frac{10}{3}}$

Figure 5: Gaussian Quadrature Nodes and Weights, [5],p.235

(Adams-Bashforth-Moulton formulas) Verify that the numerical integration formulas

a. $$\int_t^{t+h} g(s)\,ds \approx \frac{h}{24}\left[55g(t) - 59g(t-h) + 37g(t-2h) - 9g(t-3h)\right]$$

b. $$\int_t^{t+h} g(s)\,ds \approx \frac{h}{24}\left[9g(t+h) + 19g(t) - 5g(t-h) + g(t-2h)\right]$$

are exact for polynomials of third degree. *Note:* These two formulas can also be derived by replacing the two integrands g with two interpolating polynomials from Chapter 4 using nodes $(t, t-h, t-2h, t-3h)$ or nodes $(t+h, t, t-h, t-2h)$, respectively.

Figure 6: [5],p.241

Gaussian numerical integration is not as simple to use as are the trapezoidal and Simpson rules, partly because the Gaussian nodes and weights do not have simple formulas and also because the error is harder to predict. Nonetheless, the increase in the speed of convergence is so rapid and dramatic in most instances that the method should always be considered seriously when one is doing many integrations. Estimating the error is quite difficult, and most people satisfy themselves by looking at two or more successive values. If n is doubled, then repeatedly comparing two successive values, I_n, and I_{2n}, is almost always adequate for estimating the error in I_n

$$I - I_n \approx I_{2n} - I_n \; .$$

This is somewhat inefficient, but the speed of convergence in 1,, is so rapid that this will still not diminish its advantage over most other methods.

5.1 Other Gaussian quadrature rules

Gauss-Kronrod, Curtis-...

6 Integrals with Singularities

If either the interval of integration is unbounded or the function of integration is unbounded, then special procedures must be used to obtain accurate approximations to the integrals. One approach for handling a singularity in the function of integration is to change variables to remove the singularity and then use a standard approximation technique.

An important case where Gaussian formulas have an advantage occurs in integrating a function that is infinite at one end of the interval. The reason for this advantage is that the nodes in Gaussian quadrature are always *interior* points of the interval. Thus, for example, in computing

$$\int_0^1 \frac{\sin x}{x}\, dx$$

we can safely use the statement $y \leftarrow \sin x/x$ with a Gaussian formula because the value at $x = 0$ will not be required. More difficult integrals such as

$$\int_0^1 \frac{\sqrt[3]{x^2 - 1}}{\sqrt{\sin(e^x - 1)}}\, dx$$

can be computed directly with a Gaussian formula in spite of the singularity at 0. Of course, we are referring to integrals that are well defined and finite in spite of a singularity. A typical case is

$$\int_0^1 \frac{dx}{\sqrt{x}}$$

7 Adaptive method

8 What have not been covered?

In this script we have not considered the following topics.

i) Rational Function Approximation, see [4], Section 8.4.

ii) Trigonometric Polynomial Approximation, see [4], Section 8.5.

9 Survey of Methods and Software

In this chapter we considered approximating data and functions with elementary functions. The elementary functions used were polynomials, rational functions, and trigonometric polynomials. We considered two types of approximations, discrete and continuous. Discrete approximations arise when approximating a finite set of data with an elementary function. Continuous approximations are used when the function to be approximated is known.

Discrete least squares techniques are recommended when the function is specified by giving a set of data that may not exactly represent the function. Least squares fit of data can take the form of a linear or other polynomial approximation or even an exponential form. These approximations are computed by solving sets of normal equations, as given in Section 8.1.

If the data are periodic, a trigonometric least squares fit may be appropriate. Because of the orthonormality of the trigonometric basis functions, the least squares trigonometric approximation does not require the solution of a linear system. For large amounts of periodic data, interpolation by trigonometric polynomials is also recommended. An efficient method of computing the trigonometric interpolating polynomial is given by the fast Fourier transform.

When the function to be approximated can be evaluated at any required argument, the approximations seek to minimize an integral instead of a sum. The continuous least squares polynomial approximations were considered in Section 8.2. Efficient computation of least squares polynomials lead to orthonormal sets of polynomials, such as the Legendre and Chebyshev polynomials. Approximation by rational functions was studied in Section 8.4, where Padé approximation as a generalization of the Maclaurin polynomial and its extension to Chebyshev rational approximation were presented. Both methods allow a more uniform method of approximation than polynomials. Continuous least squares approximation by trigonometric functions was discussed in Section 8.5, especially as it relates to Fourier series.

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