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Numerical Differentiation and Integration

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Summary: There are several reasons why numerical differentiation and integration are used. The function that integrates $f(x)$ can be known only in certain places, which is done by taking a sample. Some supercomputers and other computer applications sometimes need numerical integration for this very reason. The formula for the function to be integrated may be known, but it may be difficult or impossible to find the antiderivation that is an elementary function. One example is the function $f(x)=\exp \left(-x^{2}\right)$, an antiderivation that cannot be written in elementary form. It is possible to find antiderivation symbolically, but it is much easier to find a numerical approximation than to calculate antiderivation (anti-derivative). This can be used if antiderivation is given as an unlimited array of products, or if the budget would require special features that are not available to computers.

Keywords: numerical integration, numerical differentiation, Newton-Cotes formulas, Special cases of NewtonCotes formulas.

## 1. INTRODUCTION

Numerical analysis is a branch of numerical mathematics that deals with finding and improving algorithms for numerical calculation of values related to mathematical analysis, such as numerical integration, numerical derivation and numerical solution of differential equations. An integral part of numerical analysis is the evaluation of method errors (algorithms) on two levels - analysis of errors of the method itself, and analysis of errors that occur due to evaluation, and are related to computer architecture.

Numerical differentiation and integration play a very important role in data processing, especially in the incorporation of curves and surfaces. Although there are many different formulas for numerical
differentiation and integration, for example, the divisive difference formula for numerical differentiation, the Newton-Cotes formula and Gaussian quadrature rules, etc., for numerical integration, they have in common the fact that these formulas are based directly on polynomials, so it is assumed that a higher order of approximation can be achieved only if the data comes from very smooth functions.[1]
The needs for numerical solution of mathematical problems are multiple. For some problems, it is proved that the analytic solution (the solution written using elementary functions) does not exist - for example the integral solution $\int e^{x^{2}} d x$ it is impossible to write using elementary functions. And still, definite integral $\int_{a}^{b} e^{x^{2}} d x$ represents a concrete, uniquely defined surface. Up to that value, which is widely used e.g. in statistics, it is possible to arrive only by numerical methods.[2]

In addition, numerical methods are often used to determine solutions to mathematical problems that, due to their size, through a standard solution procedure, would take too long - for example, when it is necessary to solve a system of 10,000 equations with 10,000 unknowns. Finally, numerical methods are unavoidable in approximation calculus, when approximations (and estimates of associated errors) replace the actual value of a function that is impossible or too difficult to arrive at. These are methods such as the finite element method or cubic splines, which approximate the behavior of an unknown function about which we know only a finite number of values, most often obtained by measurements.[3]

## 2. NEEDS FOR NUMERICAL INTEGRATION

Numerical integration is used to determine the approximate value of a particular integral of the given function. A large number of integrals do not have an analytical solution, so if we do their value is needed, we must look for it by some numerical method. It also often occurs a situation when we do not know the analytical form of the function to be integrated, but we do set its values to finally many points of the observed integration interval. We will analyze the numerological methods of determining a definite integral with a finite real boundaries $(a, b)$ and the subintegral function $f(x)$ which is a real function of one variable.[4]

A definite integral, in the case of a function that takes only positive values, we can interpreted as an area bounded by the $x$-axis, vertical straight lines for $x=a$ and $x=b$ and with upper sides by the function
$f(x)$. When searching for the integral of the function $f(x)$ in the range from $a$ to $b$ :

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

take the values of the function at $N+1$ points: $a=x_{0}<x_{1}<x_{2}<x<\ldots<x_{N-1}<x_{N}=b$ arranged between points $a$ and $b$. We will denote the values of the function at these points by $y_{0} y_{1, \ldots}, y_{N}$, where is $y_{i}=f\left(x_{i}\right)$.

A set of points defined in this way is called a division interval $(a, b)$. The distance between the points $x_{i}$ and points $x_{i+1}$ we will mark with $\Delta x_{i} \cdots x_{i+1}-x_{i}$. If all adjacent points are at the same distance, ie if $\Delta x_{i}$ does not depend on the index $i$ then we call the division uniform and instead of $\Delta x_{i}$ we write only $\Delta x$. All data related to the division of the interval and the values of the function in the division points are most easily shown in the table:

| $x$ | $x_{0}$ | $x_{1}$ | $\ldots$ | $x_{N}$ |
| :--- | :--- | :--- | :--- | :--- |
| $f(x)$ | $y_{0}$ | $y_{1}$ | $\ldots$ | $y_{N}$ |

The integral of the function in the range from $a$ to $b$ can be written as the sum of the integrals over all intervals of interval division $(a, b)$ :

$$
\int_{a}^{b} f(x) d x=\sum_{i=0}^{N-1} \int_{x i}^{x i+1} f(x) d x
$$

## 3. CALCULATION OF THE VALUE OF A GIVEN INTEGRAL

Numerical integration is used in cases where:

- subintegral function given in a table,
- determination of primitive function complicated,
- it is impossible to determine the primitive function of a subintegral function, and the numerical value of a definite integral exists ...[5]

Numerical integration deals with procedures for approximately calculating the value of a given integral:

$$
I(f ; a, b)=\int_{a}^{b} f(x) d x
$$

based on a series of values $f$. It is assumed that $f$ is continuous on the interval $[a, b]$.
Formulas used to numerically calculate simple integrals are called quadrature formulas, whose form is:

$$
Q_{n}(f ; a, b)=\sum_{k=1}^{n} A_{k} f\left(x_{k}\right)
$$

If $x_{1}=a$ and $x_{n}=b$, the quadrature formula is of the closed type, and in other cases it is of the open type.[6]

The selection of nodes and weight coefficients is done so that the quadrature formula $Q_{n}(f ; a, b)$ represents the best possible approximation for $I(f ; a . b)$. Numerical integration error $E_{n}(f)$ is the difference:

$$
E_{n}(f)=I(f ; a, b)-Q_{n}(f ; a, b)=\int_{a}^{b} f(x) d x-\sum_{k=1}^{n} A_{k} f\left(x_{k}\right)
$$

and is called the remainder of the quadrature formula. One way to estimate the error $E_{n}(f)$ is by using an algebraic degree of accuracy.[7]
Definition: The quadrature formula $Q n(f ; a, b)$ is of algebraic degree of accuracy p if $E_{n}\left(x^{i}\right)=0, i=0,1, \ldots, p$

$$
\text { i } E_{n}\left(x^{p+1}\right) \neq 0
$$

When determining $x_{k}$ and $A_{k}(k=1,2, \ldots n)$, the following approaches are common:

- nodes $x_{k}$ are known and fixed in advance, and the coefficients $A_{k}$ are determined from the conditions to obtain the maximum degree of accuracy, ie. that $E_{n}\left(x^{i}\right)=0$, za $i=0,1, \ldots, n-1$.
the coefficients $A_{k}$ and the nodes $x_{k}$ are determined so that $E_{n}\left(x^{i}\right)=0$, za $i=0,1, \ldots, 2 n-1$.


### 3.1. Newton-Cotes formulas

Newton-Cotes formulas are quadrature formulas with nodes that are predefined. The weight coefficients are determined by replacing the subintegral function with its interpolation polynomial (Lagrange) whose integration is then performed directly.[8] The quadrature Newton-Cotes formula has the following form:

$$
\int_{a}^{b} f(x) d x=(b-a) \sum_{k=0}^{n} H_{k} f\left(x_{k}\right)+E_{n}(f)
$$

where are they:

$$
\begin{gathered}
x_{1}, x_{2}, \ldots, x_{n} \in[a, b], x_{0}=a, x_{k}=x_{0}+h k, h=\frac{b-a}{n} \\
p=\frac{x-x_{0}}{h}, p^{[n+1]}=p(p-1) \ldots(p-n) \\
H_{k}=\frac{(-1)^{n-k}}{n!n}\binom{n}{k}_{0}^{n} \int_{0}^{[n+1]} \frac{p^{[n+1}}{p-k} d p, k=0,1, \ldots, n-\text { Cotes coefficients } \\
E_{n}(f)-\text { corresponding error }
\end{gathered}
$$

Newton-Cotes formulas can be useful if given function values at equidistant points. Also, there are even more convenient methods that are used if we do not have equally distant points, such as the Gaussian quadrature and the Clenshaw-Curtis quadrature, but we will not address them in this paper.[9]

### 3.2. Special cases of Newton-Cotes formulas

The special case that we will consider is the simplest, and that is the center point rule, which is an example of an open-type formula. After that we deal with the trapezoidal rule and the last Simposon rule which are of the closed type. for each of the above cases, we also list the generalized form, which we obtain by dividing the integration segment into subsegments of equal length by separately applying the quadrature formula and summing the obtained results. We will also estimate the error of approximation of each formula by applying Theorems, and finally demonstrate all cases on the same example for a better comparison.[10]

$$
\int_{a}^{b} f(x) d x=h\left(\frac{f\left(x_{0}\right)}{2}+f\left(x_{1}\right)+\ldots+f\left(x_{n-1}\right)+\frac{f\left(x_{n}\right)}{2}\right)-\frac{(b-a)^{3}}{12 n^{2}} f^{\prime \prime}(\xi)
$$

### 3.2.1. Generalized Simpson's formula

$$
\begin{gathered}
\int_{a}^{b} f(x) d x=\frac{h}{3}\left(f\left(x_{0}\right)+4 f\left(x_{1}\right)+2 f\left(x_{2}\right)+4 f\left(x_{3}\right)+\ldots+2 f\left(x_{2 n-2}\right)+4 f\left(x_{2 n-1}\right)+f\left(x_{n}\right)\right)+E(f) \\
E_{3}(f)=-\frac{(b-a)^{5}}{2880 n^{4}} f^{(4)}(\xi), \xi \in(a, b)
\end{gathered}
$$

In this case, the interval $[a, b]$ is divided into $2 n$ subintervals, a $h=\frac{b-a}{2 n}$.

## 4. NUMERICAL DIFFERENTIATION

Numerical differentiation is the process of finding the numerical value of a derivative of a given function at a given point. In general, numerical differentiation is more difficult than numerical integration. This is because while numerical integration requires only good continuity properties of the function being integrated, numerical differentiation requires more complicated properties such as Lipschitz classes.[11]

Let the values of the function be given $y_{i}=f\left(x_{i}\right)$ in dots $x_{i} \in[a, b]$. Excerpts $y^{\prime}=f^{\prime}(x)$ i $y^{\prime \prime}=f^{\prime \prime}(x)$ at the mentioned points can be determined using Newton-Gregory formulas:

$$
\begin{gathered}
y^{\prime}(x)=\frac{1}{h}\left(\Delta y_{0}-\frac{\Delta^{2} y_{0}}{2}+\frac{\Delta^{3} y_{0}}{3}-\frac{\Delta^{4} y_{0}}{4}+\ldots+(-1)^{n-1} \frac{1}{n} \Delta^{n} y_{0}\right) \\
y^{\prime \prime}(x)=\frac{1}{h^{2}}\left(\Delta^{2} y_{0}-\Delta^{3} y_{0}+\frac{11}{12} \Delta^{4} y_{0}-\frac{5}{6} \Delta^{5} y_{0}+\ldots\right)
\end{gathered}
$$

The error of the first statement is determined by the formula:

$$
R(x) \approx \frac{(-1)^{k} \Delta^{k+1} y_{0}}{h(k+1)}
$$

## 5. STABILITY OF SOLVING NUMERICAL METHODS

A numerical solution is said to be stable if errors occur during numerical solving do not increase during the solving process. There is stability of particular importance for numerical methods based on iterative addressing. In them, the condition of stability is related to the notion that the error between the two consecutive solutions during iterations must tend to zero. The method is stable if error does not diverge during the resolution process. One of the most widespread driveway researching the stability of the solution is the so-called. Neumann's method.

## 6. CONCLUSION

Modern teaching of mathematics cannot be imagined without the application of modern educational technology. In modern organized teaching of mathematics, the process of acquiring mathematical knowledge by applying modern educational technology, in addition to perceptions and ideas acquired through observation, includes very intense intellectual activities, abstract thinking, which should be especially taken into account. This means that the use of modern educational technology is in the function
of the development of mathematical thinking and the successful adoption of mathematical concepts only if it ensures and encourages appropriate thinking activities of students. The application of modern educational technology in the realization of mathematical contents should create such a climate in the classroom that students gladly accept their obligations and effectively adopt the planned contents.

The main goal of each numerical method is to solve one or a system of equations that cannot be solved analytically. The foundation of every numerical method lies in the so-called. discretization of the domain in which the solution of the equation is desired. The starting point of each numerical method is a mathematical model, ie. a set of equations that need to be solved, together with the initial and boundary conditions in order to obtain an unambiguous solution. Mathematical models are usually simplified compared to the original starting balance equations for easier numerical solution. Usually, a general mathematical model that can cover all cases is never set, but models are developed on a case-by-case basis.

The main task of the paper is to process methods for numerical solution of certain integrals. Numerical methods are used when a primitive function cannot be obtained using standard methods or when a subintegral function is defined at only a few points.

This paper describes Newton-Cotes formulas for numerical integration and errors introduced using approximations. Newton-Cotes formulas are the most direct technique for calculating certain integrals by numerical methods. The Newton-Cotes method approximates a function of a regression interval or a series of equal intervals by polynomials of different degree. The most commonly used Newton - Cotes formulas are the Trapezoid (approximation by a two-point Lagrange polynomial) and Simpson's method (approximation by a three-point Lagrange polynomial).

Furthermore, complex Newton-Cotes formulas are described, the purpose of which is to increase the accuracy of the described methods, without increasing the complexity or degree of polynomials when introducing approximations.

Basic ideas and concepts in numerical analysis in most numerical methods a small number of general and relatively simple ideas are applied. These ideas are interconnected with some additional knowledge about the problem being solved. This chapter gives some basic general ideas behind the numerical methods for solving simpler problems, which can be part of solving a larger problem.

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