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ABSTRACT

It is noted that there are some integrals which cannot be evaluated by determining an antiderivative, and these integrals must be subjected to other techniques. Numerical integration is one such method; it provides a sum that is an approximate value for some integral types. This module's purpose is to introduce methods of numerical integration and to describe related computer programing techniques for electronically carrying out the calculations. The material is seen to require very little background or knowledge about computers and their use. Exercises are provided at various points. It is expected that users work each of these problems, as they are viewed as essential to a genuine understanding of the ideas developed. (MP)

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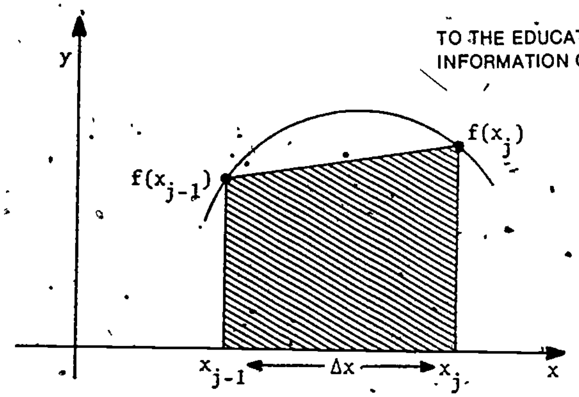
UNIT 379

ELEMENTARY TECHNIQUES OF NUMERICAL INTEGRATION AND THEIR COMPUTER IMPLEMENTATION

by Wendell L. Motter



APPLICATIONS OF ELEMENTARY CALCULUS TO COMPUTER SCIENCE

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ELEMENTARY TECHNIQUES OF NUMERICAL INTEGRATION AND THEIR COMPUTER IMPLEMENTATION

by

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Intermodular Description Sheet: *UMAP Unit 379*

Title: ELEMENTARY TECHNIQUES OF NUMERICAL INTEGRATION AND THEIR COMPUTER IMPLEMENTATION

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Review Stage/Date: III 3/20/80

Classification: APPL ELEM CALC/COMP SCI

Suggested Support Material: Either a mini-computer or time-sharing terminals which allow programming in BASIC will be needed.

Prerequisite Skills:
1. Calculus through the definite integral and Riemann Sums.
2. The analytic definition of the integral.

Output Skills:
1. Write programs in BASIC to calculate Riemann Sums for various functions.
2. Approximate integrals using the Trapezoidal Rule and Simpson's Rule and write programs in BASIC to do this.
3. Explain why the Trapezoidal Rule and Simpson's Rule give better approximations of most integrals than rectangle approximations.
4. Know the method of "doubling the number of subintervals" to improve approximations to definite integrals.

MODULES AND MONOGRAPHS IN UNDERGRADUATE MATHEMATICS AND ITS APPLICATIONS PROJECT (UMAP)

The goal of UMAP is to develop, through a community of users and developers, a system of instructional modules in undergraduate mathematics and its applications which may be used to supplement existing courses and from which complete courses may eventually be built.

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1. INTRODUCTION AND OVERVIEW

Throughout most of your studies in calculus, you will be concerned with the evaluation of integrals. Various techniques such as integration by parts are developed so that the antiderivative can be determined and used to calculate the precise value of an integral according to the fundamental theorem of calculus.

However, there are some integrals which can not be evaluated by determining an antiderivative. The integral

$$\int e^{-x^2}\,dx$$

which arises in probability theory is one of many examples. For such integrals, we must use other techniques, such as "numerical integration" to find approximate numerical values for such integrals.

The very definition of the integral as the limit of a Riemann sum provides one numerical method for computing a sum which approximates

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

where $f(x)$ is a bounded function in the interval $[a,b]$. Other methods are the trapezoidal rule and Simpson's rule.

The purpose of this unit is to introduce these methods of numerical integration and describe the

related programming techniques required for having a computer carry out the calculations. This unit requires very little previous background or knowledge about computers and their use.

Throughout the module, various references are cited and a complete bibliography follows the main text. Students are encouraged to pursue further readings that are suggested if they desire a deeper understanding of this material. Most importantly, students are expected to work each of the several exercises; for these are essential to a geniune understanding of the ideas developed.

2. APPROXIMATING INTEGRALS USING RIEMANN SUMS

2.1 The Left-Rectangle Method

Our first attempt to solve the problem of evaluating definite integrals involves using Riemann sums as approximations. We consider a function f defined on a closed finite interval $a \le x \le b$ and a partition $a = x_0 < x_1 < x_2 < \ldots < x_{N-1} < x_N = x_N = b$ of that interval. For each $j = 1, 2, \ldots, N$, let c_j be any point in the j^{th} subinterval of the partition,

i.e., $x_{j-1} \le c_j \le x_j$.

The Riemann sum

$$\sum_{j=1}^{N} f(c_j)\cdot(x_j - x_{j-1}) = f(c_1)\cdot(x_1 - x_0) + f(c_2)\cdot(x_2 - x_1) + \ldots + f(c_N)\cdot(x_N - x_{N-1})$$

is an approximation of the integral $\int_a^b f(x)\,dx$. The j^{th} term of this sum, $f(c_j)\cdot(x_j - x_{j-1})$, is described geometrically in Figure 1 as the area of the shaded rectangle. The approximation of the integral that is

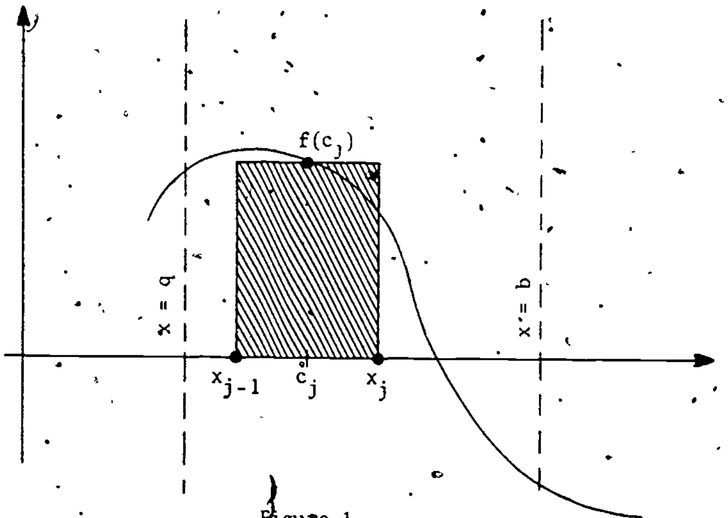


Figure 1.

determined by the partition is the sum of the areas of N rectangles of heights $f(c_j)$--this area actually is negative when $f(c_j)$ is negative--and widths $(x_j - x_{j-1})$.

In this general formula, the value of c_j in the subinterval $[x_{j-1}, x_j]$ can be chosen arbitrarily and in fact so can the x_j's in the partition. To implement this method on a computer, we need a systematic way of making these choices. One method is to choose a partition in which each subinterval has the same width as each other subinterval. This is easily accomplished by subdividing the interval $[a,b]$ whose width is $(b-a)$ into N equal subintervals each with width $(b-a)/N$. A convenient and standard notation for the quantity $(b-a)/N$ is Δx. The partition is then

$$a = x_0, \; x_1 = a + \Delta x, \; x_2 = a + 2\Delta x, \; \ldots$$
$$x_{N-1} = a + (N-1)\Delta x, \; x_N = b$$

so we have N subintervals

$$[a, a + \Delta x], \; [a + \Delta x, a + 2\Delta x],$$
$$\ldots, \; [a + (N-1)\Delta x, b]$$

each of which has length Δx.

Now if we choose c_j as the left endpoint of each of these subintervals so that

$$c_1 = a, \; c_2 = a + \Delta x, \; \ldots, \; c_N = (N-1)\Delta x$$

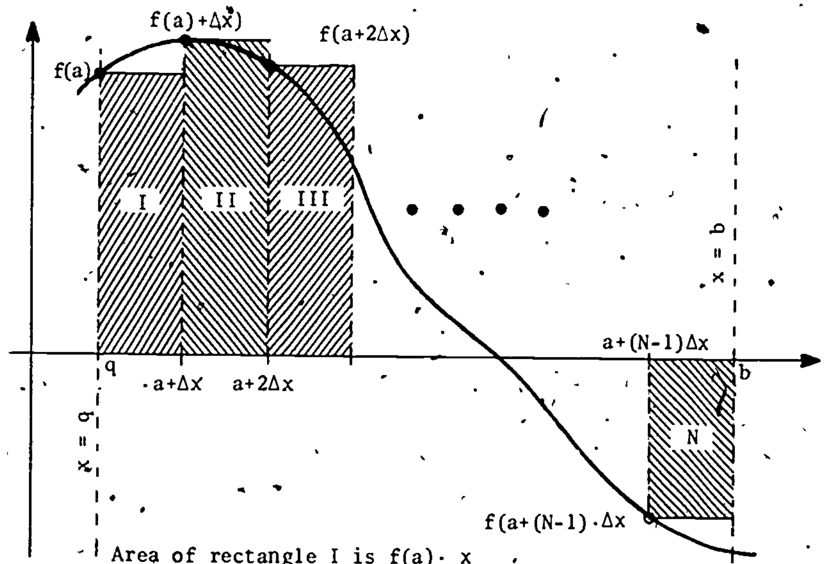
then we can form a Riemann sum approximating the integral called the *left-rectangle approximation*. It is given by the following expression:

$$f(a)\Delta x + f(a + \Delta x)\Delta x$$
$$+ f(a + 2\Delta x)\Delta x + \ldots + f(a + (N-1)\Delta x)\Delta x.$$

This can be simplified to

(1) $$[f(a) + f(a + \Delta x) + \ldots + f(a + (N-1)\Delta x)]\Delta x.$$

This approximation is shown in Figure 2.



Area of rectangle I is $f(a)\cdot x$
Area of rectangle II is $f(a+\Delta x)\cdot\Delta x$
Area of rectangle III is $f(a+2\cdot\Delta x)\cdot\Delta x$
⋮
Area of rectangle N is $\underline{f(a+(N-1)\Delta x)\cdot\Delta x}$
Sum of above is Formula (1)

Figure 2.

Let us use the left-rectangle method to approximate the integral

$$\int_0^1 \frac{1}{1+x^2}\,dx,$$

which in fact we know to be

$$\arctan(1) - \arctan(0) = \frac{\pi}{4} = .78539.$$

Here $f(x) = 1/(1 + x^2)$.

Suppose we use $N = 4$. Since $b = 1$ and $a = 0$ we have $\Delta x = 1/4$. Thus the partition is

$$a = 0,\ x_1 = 1/4,$$

$$x_2 = 1/2,\ x_3 = 3/4,\ b = 1$$

and the approximation (1) is

$$[f(0) + f(1/4) + f(1/2) + f(3/4)] \cdot 1/4$$

$$= [1 + 16/17 + 4/5 + 16/25] \cdot 1/4$$

$$= [1 + .941 + .800 + .640] \cdot 1/4$$

$$= .845.$$

Although we intend to use the computer to find better approximations by increasing the value of N, it is important that you understand how to use these formulas with hand calculations also.

Now we are ready to devise a simple program (which can easily be translated into a language like BASIC) that will compute an approximation to an integral by the left-rectangle method. As Formula (1) indicates, we need to have x range through the values of a, $a + \Delta x$, $a + 2\Delta x$, ..., $a + (N-1)\Delta x$, i.e., x ranges from a to $a + (N-1)\Delta x$ in steps of Δx. We need to calculate f(x) for each such x, and add up these terms to form a sum S which we then multiply by Δx to compute the left-rectangle approximation. Suppose we use the computer variable D (for "delta") to represent Δx; the following

program is probably what you would have designed. In this example program, we use the function $f(x) = 1/(x^2+1)$ which we define in the first line of code.

Example Program 1

```
100 DEF FNA (X) = 1/(X↑2 + 1)
110 INPUT A, B, N
120 LET D = (B-A)/N
130 LET S = 0
140 FOR X = A to (A + (N-1)*D) STEP D
150    LET S = S + FNA (X)
160 NEXT X
170 PRINT S*D; "IS THE LEFT-RECTANGLE APPROX."
180 END
```

Note that when the INPUT A, B, N, instruction is exectued, the computer will request 3 numerical values for A, B, and N respectively. (In an interactive BASIC session, these must be separated by commas when typed in.) Line 170 computes S·D and prints this value out along with the descriptive phrase enclosed in quotes.

If we increase the number of subintervals by using larger values of N, we expect to obtain a better approximation to the integral since the Δx will be smaller and the rectangle more closely matched to the function. This is so because the left-rectangle approximation, being a Riemann sum, tends to the value of the integral as Δx is made smaller.

Now, in Example Program 1, we used $f(x) = 1/(x^2+1)$ which has antiderivative arctan (x). Thus, in this case we can determine the exact value of the integral

$$\arctan(B) - \arctan(A)$$

and compare it with our numerical approximation.

We can make such a comparison anytime we work with an f(x) for which we know the antiderivative. For instance, we could do this with $f(x) = 4x^3 - 3x^2 + 2x - 7$ whose antiderivative is $x^4 - x^3 + x^2 - 7x$. We can easily modify the code of our Example Program 1 to handle this new function by changing line 100 to

```
100  DEF FNA (x) = 4*x↑3 - 3*x↑2 + 2*x - 7
```

To make it easy to compare our numerical approximation with the exact value we can add a line or two of code to calculate the exact value from the antiderivative and then print out that value. We could do this by adding the line

```
175  PRINT B↑4 - B↑3 + B↑2 - 7*B - A↑4 + A↑3 - A↑2 + 7*A
```

(Note this is not the most efficient way to evaluate a polynomial, but it is straightforward and easy to write. Horner's method would be much better; see UMAP Unit 263, *Horner's Scheme and Related Algorithms*, by Werner C. Rheinboldt. If we are going to perform such an evaluation many times, we might consider such improvements.)

Now that we have the program for the left-rectangle method, we can perform many experiments. For instance, we can change the function we want to integrate. We can also vary the N (and thus the Δx) to examine the "goodness" of our method.

Exercise 1.

Run Example Program 1 for $f(x) = 4x^3 - 3x^2 + 2x - 7$ for fixed values of A and B but make N increasingly larger. Copy some of your results on notepaper including the values of A, B, N for several choices of N. Does the approximation get closer to the exact value of the definite integral?

You might have noticed that it is only necessary to calculate once the exact value of the integral for given values of N. Thus line 175 really should not be executed every time you run the program for a new N. If you plan to run many experiments, you should consider placing line 175 outside the "loop" of your changes to N, for instance,

by doing the exact evaluation before you begin any approximations. This would also help you to determine if your program is running correctly. This is a standard technique; namely, testing a program with known results.

2.2 The Right-Rectangle Method

Suppose instead of choosing c_j as the left-endpoint of each subinterval, we choose c_j as the right-endpoint of each subinterval so that $c_1 = a + \Delta x$, $c_2 = a + 2\Delta x$, $\ldots$, $c_N = a + N\Delta x = b$. Then our approximating Riemann sum becomes

$$(2)\qquad [f(a + \Delta x) + f(a + 2\Delta x) + \ldots + f(b)]\cdot \Delta x.$$

As this formula indicates, we need to have x run through the values $a + \Delta x$, $a + 2\Delta x$, $\ldots$, B, calculate $f(x)$ for each such x, and add up these terms to form a sum S which is then mulitplied by Δx to compute what is called the *right-rectangle approximation*.

Exercise 2.

Modify Example Program 1 so that the sum S is calculated as the right-rectangle approximation. Type in this modified program on a computer terminal with instruction 175 which prints out the exact value of the $\int_a^b f(x)\,dx$ for $f(x) = 4x^3 - 3x^2 + 2x - 7$. Run this for fixed values of A, B but use several increasingly larger values of N. Compare your results with those of Exercise 1. Make a hard-copy listing of your program. This should be turned in to your instructor.

---

3. THE TRAPEZOID RULE

One way to see why the left-rectangle method is somewhat crude is that the approximation on the j^{th} subinterval makes use of only the value of $f(x)$ at the left endpoint x_{j-1}. Although this is not too bad if the graph of $f(x)$ looks like the one shown in Figure 1, it is not all that good if the graph of $f(x)$ looks like the function in Figure 3.

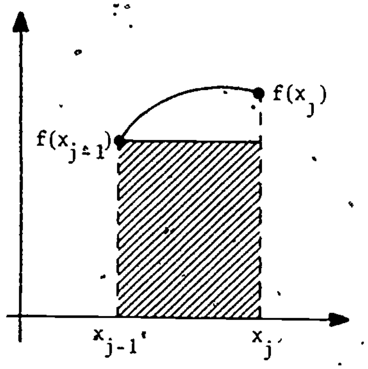


Figure 3.

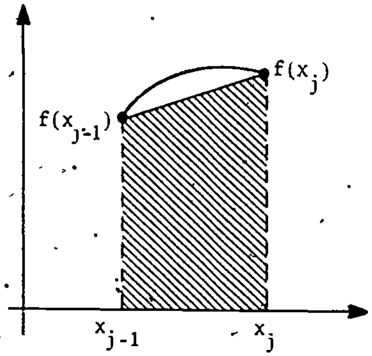


Figure 4.

One way in which the error might be reduced is illustrated in Figure 4. Here, we approximate

$$\int_{x_{j-1}}^{x_j} f(x)\,dx$$

by the integral of the function whose graph is the straight line connecting the points $(x_{j-1}, f(x_{j-1}))$ and $(x_j, f(x_j))$. As Figure 4 shows, this would mean approximating the area under the graph of $f(x)$ over the subinterval $[x_{j-1}, x_j]$ by the area of the shaded trapezoid. This is the basis for the method known as the trapezoid rule. Actually, this and other methods of numerical integration that we shall discuss follow the same approach as the left and right rectangle approximations by trying to approximate the area under the curve of $f(x)$ for each subinterval. The idea behind the trapezoid rule is to sum areas of trapezoids instead of areas of rectangles.

In general, a trapezoid can be formed by the 4 points $(x_{j-1}, 0)$, $(x_{j-1}, f(x_{j-1}))$, $(x_j, 0)$, $(x_j, f(x_j))$ as illustrated by the following diagram for the j^{th} subinterval (Figure 5). (In Figure 5 we are really using a linear function, namely the one represented by the line through $f(x_{j-1})$ and $f(x_j)$ to approximate the curve of $f(x)$ in the j^{th} subinterval.) From elementary geometry, we know the area of the trapezoid is given by

$$A = 1/2\,[f(x_{j-1}) + f(x_j)]\Delta x.$$

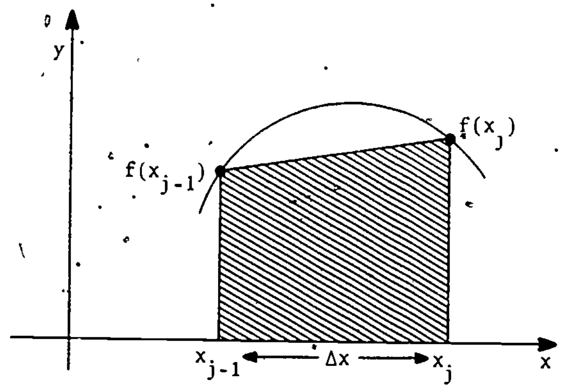


Figure 5.

Now suppose we have partitioned the interval $a \le x \le b$ into N equal subintervals of length $\Delta x = (b-a)/N$ as before. Then we will have N trapezoids similar to the one described in Figure 5. The total area of these N trapezoids over

$$a = x_0,\ (a + \Delta x) = x_1,\ \ldots,\ b = x_N$$

may be expressed as

$$\Delta x\{1/2[f(a) + f(a + \Delta x)] + 1/2[f(a + \Delta x) + f(a + 2\Delta x)]$$
$$+ \ldots$$
$$(3) \qquad + 1/2[f(a + (N-1)\Delta x) + f(b)]\}$$
$$= \Delta x\{f(a + \Delta x) + f(a + 2\Delta x) + \ldots + f(a + (N-1)\Delta x)\}$$
$$+ 1/2(f(a) + f(b))\Delta x.$$

Let us find an approximation for $\int_0^1 1/(1 + x^2)\,dx$ by means of the trapezoid rule (3). Again we use N = 4 so $\Delta x = 1/4$ and the partition is $a = 0$, $x_1 = 1/4$, $x_2 = 1/2$, $x_3 = 3/4$, $b = 1$ as when we used the left-rectangle method for this example. The approximation (3) gives

$$1/4[f(1/4) + f(1/2) + f(3/4)] + 1/4 \cdot 1/2[f(0) + f(1)]$$
$$= 1/4[16/17 + 4/5 + 16/25] + 1/8[1 + 1/2]$$
$$= 4/17 + 1/5 + 4/25 + 3/16$$
$$= .2353 + .2000 + .1600 + .1875$$
$$= .7828.$$

Compare this result for this same problem with the left-rectangle method and its result as shown on page 5.

Exercise 3.

Compute $\int_1^2 1/x\,(dx)$ by hand calculations using the trapezoid rule (3) where N = 6. Note the exact value is ln (2).

Instead of writing a program to compute the approximation by Formula (3), we shall try to write this in another form. You should recognize that (3) is just the right-rectangle approximation

$$(2) - f(b)\Delta x + 1/2[f(a) + f(b)]\Delta x.$$

Now the quantity

$$\{- f(b)\Delta x + 1/2[f(a) + f(b)]\Delta x\}$$

can be simplified to

$$1/2[f(a) - f(b)]\Delta x.$$

This means that if the approximating sum (2) computed by the right-rectangle rule is adjusted by addition of the term $1/2[f(a) - f(b)]\Delta x$ then we have the trapezoid rule.

Thus the trapezoid rule is about as easy to program as the rectangle rules. In fact we can take the program for computing the approximating sum by the right-rectangle rule and insert additional instructions that compute $1/2[f(a) - f(b)]\Delta x$ and then add this term to the right-rectangle approximating sum. A complete program for doing this is now given. Does your solution to Exercise 2 resemble this?

Example Program 2

```
100 DEF FNA(X) = 4*X↑3 - 3*X↑3 + 2*X - 7
110 INPUT A, B, N
120 LET D = (B-A)/N
130 LET S = 0
140 FOR X = (A + D TO) TO B STEP D
150     LET S = S + FNA (X)
160 NEXT X.
170 LET S1 = S*D
175 LET S2 = S1 + D*(FNA(A) - FNA(B))/2
180 PRINT S2; "IS TRAPEZOID APPROX."
185 PRINT S1; "IS RIGHT RECTANGLE APPROX."
190 END
```

Here we use line 185 to print out S1, the right-rectangle approximation so we can compare this with the result from the trapezoid method.

Exercise 4.

Type in Example Program 2 at a computer terminal. RUN this program for fixed values of A, B and increasingly larger values of N. Copy down on notebook paper the results from these runs including your input values of A, B, N. What is the smallest value of N that gives the *exact* value of the integral for A = 0, B = 1? How does the trapezoid rule compare with the previous methods? Turn in your solution for this exercise to your instructor.

Let's review what we have done so far in computing approximations to definite integrals. Our first method was derived directly from the definition of the definite integral. The left and right rectangle approximations consist in approximating our given function for each small subinterval by a constant (either the value of the function at the left endpoint or its value at the right endpoint). The approximation to f(x) obtained by piecing together all of these constant functions for a given subdivision of the interval $[a,b]$ is called a step function, and the corresponding approximating sum (left or right) is actually the integral of this step function. This is illustrated by the following diagram with a subdivision of 5 points (Figure 6).

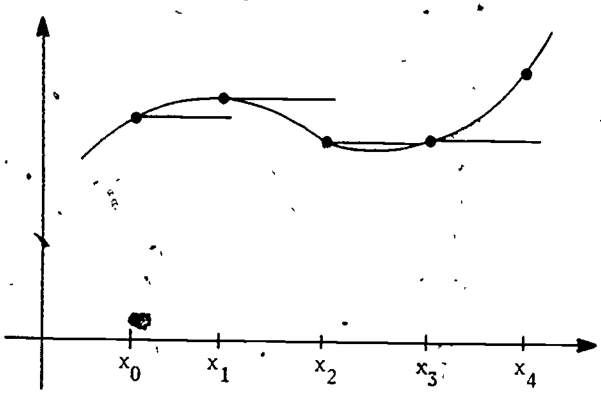


Figure 6.

The trapezoidal rule used a linear approximation to $f(x)$ on each subinterval. The approximating function obtained by piecing together all of the linear pieces for a given subdivision of $[a,b]$ is called piecewise linear, and the approximating trapezoidal sum is actually the integral from a to b of such a piecewise linear function. The previous exercises should have demonstrated to you that the trapezoid method gives a better approximation for each N than the rectangle methods.

This illustrates how complicated functions are approximated on suitably small portions of their domains by simpler functions, and the desired analysis is done with these simpler functions. Polynomial functions are the best examples of simple functions because their values are easily computed and there are simpler formulas for integrating and differentiating these. Actually, a constant function is a polynomial function of degree 0 and linear function is a polynomial function of degree one; thus, we might expect greater accuracy (or better fit) by using second-degree polynomial functions, such as parabolas,

to approximate $f(x)$ on suitably small subintervals and piece these together to approximate the integral of $f(x)$ over $[a,b]$.

4. SIMPSON'S RULE

This approach leads to our next method of numerical integration which is called Simpson's Rule and approximates the area under the curve of $f(x)$ over two adjacent subintervals by means of a parabola. The approximation for the integral

$$\int_{x_{j-1}}^{x_{j+1}} f(x)\,dx$$

is derived by passing a parabola $g_j(x)$ through the three points $(x_{j-1}, f(x_{j-1}))$, $(x_j, f(x_j))$, and $(x_{j+1}, f(x_{j+1}))$ of the adjacent subintervals $[x_{j-1}, x_j]$ and $[x_j, x_{j+1}]$. The approximation to the area under the curve of $f(x)$ over the adjacent subintervals $[x_{j-1}, x_j]$ and $[x_j, x_{j+1}]$ is given by calculating the area under the parabola $g_j(x)$ over these subintervals. This is shown in Figure 7.

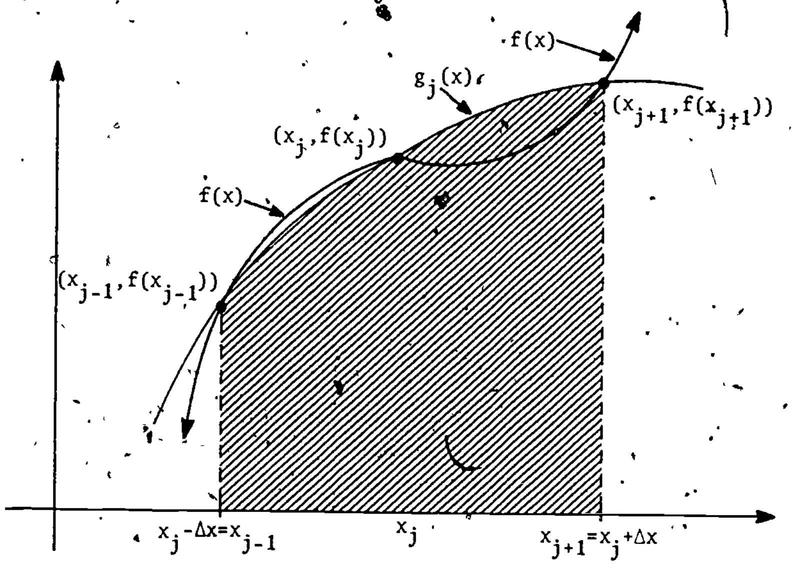


Figure 7.

Of course the overall approximation $\int_a^b f(x)\,dx$ consists of the sum of the areas for these approximations by parabolas g_j where j runs through the indices 1, 3, 5, ..., N-1. A pair of adjacent subintervals must be used as 3 points are required to uniquely determine each approximating parabola $g_j(x)$ and there must be an even number of subintervals altogether so these can be paired off. This means choices for the values of N which represents the total number of subintervals must be even. To derive a formula for Simpson's Rule to approximate $\int_a^b f(x)\,dx$, we will assume there are an even number of subintervals in the partition of [a,b] and that each of these subintervals has the same length which we denote by Δx as in previous discussions. Observe as Figure 7 indicates that $x_{j-1} = x_j - \Delta x$ and $x_{j+1} = x_j + \Delta x$.

First, let us derive a formula for the approximation to

$$\int_{x_j-\Delta x}^{x_j+\Delta x} f(x)\,dx$$

using these ideas. Let us assume the parabola $g_j(x)$ has the form $g_j(x) = ax^2 + bx + c$. The area under the parabola is

$$\int_{x_j-\Delta x}^{x_j+\Delta x} (ax^2 + bx + c)\,dx$$

$$= 1/3\, ax^3 + bx^2/2 + cx \Big|_{x_j-\Delta x}^{x_j+\Delta x}$$

By substitution and algebraic simplification, this equals

(4-a) $\quad 1/3 \cdot \Delta x \cdot (6ax_j^2 + 6bx_j + 2a\Delta x^2 + 6c)$.

A computational formula should involve the values of the original function f(x) at the points $x_j - \Delta x$, x_j, and $x_j + \Delta x$; this will occur through the determination of the coefficients a, b, and c. Finding the solution of the three equations $f(x_{j-1}) = g(x_{j-1})$, $f(x_j) = g(x_j)$, and $f(x_{j+1}) = g(x_{j+1})$ is one technique for calculating a, b,

and c. Appendix B contains a more detailed discussion of this and the general method of determining coefficients of the polynomial $p(x) = a_n x^n + a_{n-1}x^{n-1} + \ldots + a_1 x + a_0$ which approximates f(x) and passes through n+1 points $(x_1, f(x_1)), \ldots, (x_{n+1}, f(x_{n+1}))$ of the curve for f(x).

An easier approach is to observe that

$$g_j(x_j - \Delta x) = a(x_j - \Delta x)^2 + b(x_j - \Delta x) + c$$

$$= a(x_j^2 - 2\Delta x\, x_j + \Delta x^2) + b(x_j - \Delta x) + c$$

and likewise

$$g_j(x_j + \Delta x) = a(x_j^2 + 2\Delta x x_j + \Delta x^2) + b(x_j + \Delta x) + c.$$

Therefore,

$$g_j(x_j - \Delta x) + g_j(x_j + \Delta x)$$

$$= a(2x_j^2 + 2\Delta x^2) + b(2x_j) + 2c$$

so that if we add

$$4g_j(x_j) = 4ax_j^2 + 4bx_j + 4c$$

to this, we obtain the expression enclosed by parentheses in Formula (4-a), i.e.,

$$g_j(x_j - \Delta x) + 4g_j(x_j) + g_j(x_j + \Delta x)$$

$$= 6ax_j^2 + 6bx_j + 2a\Delta x^2 + 6c.$$

This means

$$\int_{x_j-\Delta x}^{x_j+\Delta x} g_j(x)\,dx$$

$$= 1/3\Delta x\ (g_j(x_j - \Delta x) + 4g_j(x_j) + g_j(x_j + \Delta x)).$$

Finally,

(4-b) $$\int_{x_j-\Delta x}^{x_j+\Delta x} g_j(x)\,dx$$

$$= 1/3\Delta x\ (f(x_j - \Delta x) + 4f(x_j) + f(x_j + \Delta x)).$$

Since $g_j(x_j - \Delta x) = f(x_j - \Delta x)$, $g_j(x_j) = f(x_j)$, and $g_j(x_j + \Delta x) = f(x_j + \Delta x)$ by construction.

If we add up the areas under these approximating parabolas for all nonoverlapping pairs of adjacent sub-intervals, i.e., $[x_0, x_1]$ with $[x_1, x_2]$, $[x_2, x_3]$ with $[x_3, x_4]$, $[x_4, x_5]$ with $[x_5, x_6]$, ..., $[x_{n-2}, x_{n-1}]$ with $[x_{n-1}, x_n]$, then we obtain the sum of these approximating areas from (4-b) as

$$\begin{aligned}(5)\quad &\Delta x/3[f(x_0) + 4f(x_1) + f(x_2)]\\ &+ \Delta x/3[f(x_2) + 4f(x_3) + f(x_4)]\\ &+ \ldots\\ &+ \Delta x/3[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)]\end{aligned}$$

An alternative way to write Formula (5) is

$$\int_a^b f(x)\,dx = \Delta x/3[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)].$$

Let us apply Formula (5) for Simpson's Rule to approximate $\int_0^1 1/(1 + x^2)\,dx$. For comparison with the left-rectangle and trapezoid methods, we will again use $N = 4$ so $\Delta x = 1/4$ and the partition is $a = 0$, $x_1 = 1/4$, $x_2 = 1/2$, $x_3 = 3/4$, $b = 1$ as before. Now Formula (5) gives

$$\begin{aligned}&1/4 \cdot 1/3[f(0) + 4\cdot f(1/4) + f(1/2)]\\ &+ 1/4 \cdot 1/3[f(1/2) + 4\cdot f(3/4) + f(1)]\\ &= 1/4 \cdot 1/3[1 + 4 \cdot 16/17 + 4/5]\\ &+ 1/4 \cdot 1/3[4/5 + 4 \cdot 16/25 + 1/2]\\ &= 1/3[1/4 + 16/17 + 1/5 + 1/5 + 16/25 + 1/8]\\ &= 1/3[.2500 + .9412 + .2000 + .2000 + .6400 + .1250]\\ &= 1/3\ [2.3562]\\ &= .78.\end{aligned}$$

This is illustrated by Figure 8.

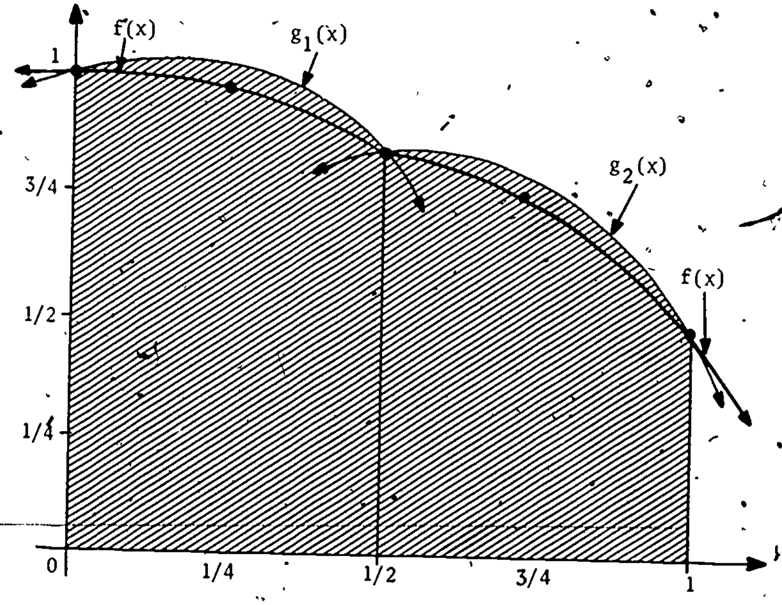


Figure 8.

Figure 8 indicates how closely the parabolas $g_1(x)$ and $g_2(x)$ approximate the curve $y = 1/(1+x^2)$ over the two pairs of subintervals and the computations illustrate that for about the same amount of effort as the trapezoid formula, Simpson's Rule gives much better accuracy. Another example which compares Simpson's Rule and the trapezoid rule is given in Shenk, p. 375.

Consider now a function whose graph over the pair of adjacent subintervals $[x_{j-1}, x_j]$ and $[x_j, x_{j+1}]$ behaves as indicated by Figure 9(a). Here the graph of the quadratic function $p(x)$ through the points corresponding to x_{j-1}, x_j, and x_{j+1} is a poor approximation to the graph of $f(x)$. This is an excellent illustration of how Simpson's Method can be made increasingly accurate by successive doubling of the number of points in the

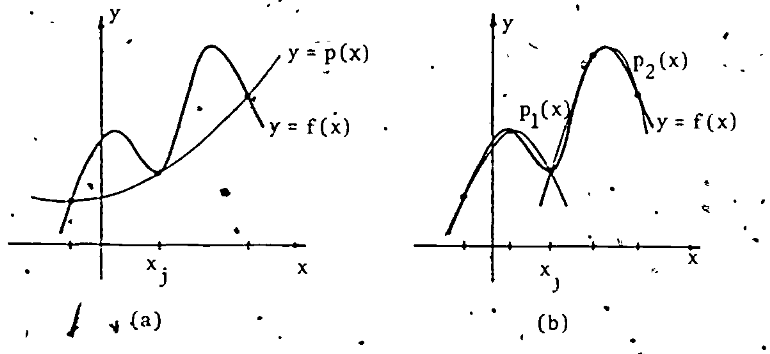


Figure 9.

subdivision of the interval [a,b] of integration (this procedure will be discussed in more detail in the next section). As Figure 9(b) illustrates, when the original pair of subintervals is subdivided into 2 pairs of subintervals, then a pair $p_1(x)$, $p_2(x)$ of quadratic functions is used to approximate f(x) and gives a closer fit to the graph. Note that in this example, the trapezoid method would still not give as good an approximation. This can be seen by drawing four line segments to connect pairs of adjacent points on the graph of f(x) since as you should recall, the trapezoid method would use such a piecewise linear approximation.

Now to implement Formula (5) on a computer, we need a computational routine whereby x ranges through the middle point of each pair of nonoverlapping adjacent subintervals so that the quantities $f(x - \Delta x) + 4f(x) + f(x + \Delta x)$ can be computed and summed. To be precise, x must range through the values $x_1, x_3, x_5, \ldots, x_{N-1}$ of our partition since the pairs of subintervals are $[x_0, x_1]$ with $[x_1, x_2]$, $[x_2, x_3]$ with $[x_3, x_4]$, ..., $[x_{N-2}, x_{N-1}]$ with $[x_{N-1}, x_N]$. Now using the uniform width Δx for such a partition means $x_1 = a + \Delta x$, $x_3 = a + 3\Delta x$, $x_5 = a + 5\Delta x$, ..., $x_{N-1} = a + (N-1)\Delta x$, i.e., x varies from $a + \Delta x$ to $a + (N-1)\Delta x$ in steps of $2 \cdot \Delta x$. Then we can use a summing

vairable S to add the quantities $f(x - \Delta x) + 4f(x) + f(x + \Delta x)$ for each x. Finally, according to Formula (5), S is multiplied by $\Delta x/3$ to complete the computation of the sum of the areas under the parabolas.

Obviously, to have a computer routine for this calculation process we would use a FOR-NEXT loop. Again using D for Δx, we have the following Example Program 3 to calculate the approximation to the integral $\int_A^B FNA(x)\,dx$ using Formula (5) for Simpson's Rule. Here again FNA(x) = $4x^3 - 3x^2 + 2x - 7$, but any function FNA(x) can be defined for any function by a suitable program instruction at line 100.

EXAMPLE PROGRAM 3

```
 90  SET DIGITS 10
100  DEF FNA(x) = 4*x↑3 - 3*x↑2 + 2*x - 7
110  INPUT A, B, N
120  LET D = (B-A)/N
130  LET S = 0
140  FOR X = (A + D) TO (A + (N-1)*D) STEP 2*D
150      LET S = S + FNA(X - D) + 4*FNA(X) + FNA(X + D)
160  NEXT X
170  PRINT S*D/3, "IS SIMPSON'S APPROXIMATION"
180  END
```

Note the instruction in line 90 SET DIGITS 10 specified that when the computer prints numerical output this will consist of 10 digit numbers.

Exercise 7.

Type in Example Program 3 at a computer terminal. Run this program for fixed values of A, B and values of N like 2, 4, 8, 16. Remember N must be even for Simpson's Rule to work. Recall that the additional instruction given as 175 PRINT B↑4 - B↑3 + B↑2 - 7*B - A↑4 + A↑3 - A↑2 + 7*A will print the exact value of the integral $\int_A^B (4x^3 - 3x^2 + 2x - 7)dx$.

Copy down on notebook paper the results from your computer run including your input values of A, B, N. What is the smallest value of N that gives the exact value of this integral for A = 0, B = 1? How does this compare with the trapezoid rule? Turn in your results for this exercise to your instructor.

An Application

We now give an application of these approximation techniques to a practical problem. Recall that if an object is moving at velocity v(t) as a function of time t, then the distance traveled between times t = a and t = b is given by

$$\int_a^b v(t)\,dt$$

provided $v(t) \geq 0$.

For example, suppose a motorist on a two hour trip noted his speed at 10 minute intervals as 0, 57, 51, 55, 0, 62, 60, 58, 35, 60, 33, 35, and 0 miles/hour. We can estimate the distance traveled by using either the Trapezoid method or Simpson's method (since there are an odd number of equally spaced speed values) to approximate

$$\int_0^2 v(t)\,dt\ ;$$

here t is time measured in hours and 10 minutes = Δt = 1/6 hour.

If we use Simpson's method, then by Formula 5 we have

$$\frac{1}{3\cdot 6}(0 + 4\cdot 57 + 51) + \frac{1}{3\cdot 6}(51 + 4\cdot 55 + 0)$$

$$+ \frac{1}{3\cdot 6}(0 + 4\cdot 62 + 60) + \frac{1}{3\cdot 6}(60 + 4\cdot 58 + 35)$$

$$+ \frac{1}{3\cdot 6}(35 + 4\cdot 60 + 33) + \frac{1}{3\cdot 6}(33 + 4\cdot 35 + 0)$$

$$= \frac{1}{3\cdot 6}(1674)$$

= 93 miles.

5. DOUBLING THE NUMBER OF SUBINTERVALS IN PARTITIONS OF UNIFORM WIDTH

So far we have discussed three techniques of numerical integration and applied each of these to $F(x) = 4x^3 - 3x^2 + 2x - 7$ over the interval [0,1] to obtain computer calculated approximations. Because we could find the antiderivative for this example, we could compute the exact value of the integral and compare how close the approximate values were when we used different numerical techniques and larger values of N. Actually when an antiderviative can be determined, there is really no point in using techniques of numerical integration. On the other hand, suppose we want to evaluate

$$\int_{-2}^{2} e^{-x^2/2}$$

for which an antiderivative can not be calculated. Here we can not find the exact value of this integral by using antiderivatives.

We have seen that larger values of N usually give better approximations by the numerical methods and we expect this to be true theoretically since we are using Riemann Sums where x approaches 0 as N approaches infinity (see Shenk, p. 207). In actuality though, a machine created error called "round-off" error will build up as N increases and more arithmetic computations are performed by the computer since each number is represented by a finite number of digits in the computer and arithmetic computations are rounded off during machine calculations.

If we neglect the effect of round-off error which will be insignificant on most computers when accuracy to only 5 or 6 decimal places is desired, then we can simply double the value of N each time. Thus, we would compute sums S_2, S_4, S_8, S_{16}, ..., and when the difference between the value, S_N, of the approximating sum for some N and the value, S_{2N}, of the approximating sum for 2N becomes less than a specified tolerance, then the computational process would be terminated.

Suppose for example we want an approximation accurate to 0.00005 for the integral of

$$e^{-x^2/2}$$

over [-2,2]. Here we use Example Programs 2 and 3 with DEF FNA() instruction changed to DEF FNA(X) = EXP(X↑2/2) and make use of the built-in function EXP() for $e^{()}$. The following tables give the results of some computer runs.

N	Trapezoid Approx.	N	Simpson's Approx.
2	2.270671	2	2.847114
4	2.348397	4	2.374305
8	2.381347	8	2.392331
16	2.389759	16	2.3922331
32	2.391871	32	2.392572
64	2.392399	64	2.392575
128	2.392531		
256	2.392565		
512	2.392573		

We want $|S_{2N} - S_N| < 0.00005$ so 2N = 32 works for Simpson's Method while 2N = 256 is necessary for the trapezoid method. Here, we observe that 2.3925 is the approximation for

$$\int_{-2}^{2} e^{-x^2/2}$$

that is accurate to 0.00005, i.e., 4 decimal places, and is obtained by both methods.

Observe that the example programs can be used to compute approximations for the integrals of other functions by simply changing the DEF FNA() instruction. For

$$F(x) = e^{-x^2/2}$$

we used the built-in function EXP(); other built-in functions are SIN(), LOG()-natural logarithm, COS(), etc. Appendix A contains a complete list of such built-in functions available in most versions of the programming language BASIC.

<u>Exercise 8</u>

Use the trapezoid and Simpson techniques to compute sin(ln(x)) dx accurate to 0.0000005 by doubling N for successive computer runs. Here DEF FNA(x) = SIN (LOG(x)). What are the values of N required for each technique? Remember to insert the instruction 5 SET DIGITS 10.

<u>Exercise 9</u>. Since $\int_0^1 1/(1+x^2)\,dx = \text{Arctan}(1) = \pi/4$ then $4 \cdot \int_0^1 1/(1+x^2)\,dx = \pi$. Use the method of doubling the number of subintervals to find the value of π accurate to 8 decimal places. What are the values of N required for this technique? Use only Simpson's Method (Example Program 3) and the additional instruction 175 PRINT 4*S*D/3, "IS THE APPROXIMATION TO π".

Note: π = 3.14159265358979323846264...

In practice, most numerical integration techniques are carried out on a computer; and the accuracy of the approximation is usually determined by doubling the number of subintervals until two successive approximations differ by less than the prescribed tolerance. This "stopping rule", although widely used, does not always work efficiently. Consider the Figure 10; this shows that unless the number of subdivision points is large enough to require the integrand to be evaluated at points in the interval [c, c+h], very little change will be noticed between two successive approximations.

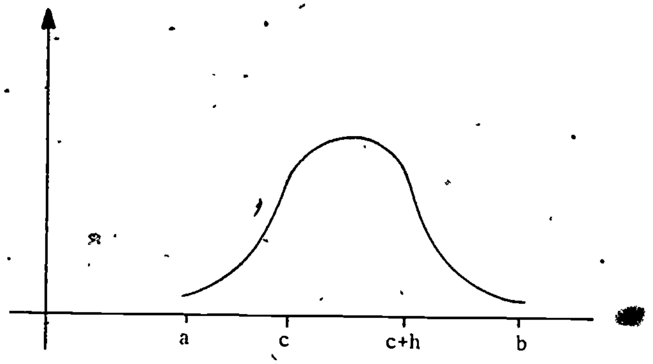


Figure 10.

There is another reason for doubling N until two successive approximations differ by less than the prescribed tolerance. If an "optimal" N were on the order of 400 for example, one would expect S_{200} and S_{202} to be very close to each other, even if neither were close enough to the correct approximation. Actually, a more elaborate computational algorithm can incorporate the computations used in the calculation of S_N when S_{2N} is computed. This approach would give a more efficient program and eliminate unnecessary duplication of computations which occurs when a straightforward program like Example Program 3 is simply repeated for N = 2, 4, 8,.... An example of such an algorithm for Simpson's Method is described by D.A. Smith (21, p. 121-122).

It is important to note that Simpson's rule requires an evenly spaced partition with an even number of subintervals. Thus, given y = F(x) if the x-values do not satisfy this criteria then the trapezoid method is the only one of these two methods that can be used. This will only occur for functions defined from experimental data as in the applications example of Section 4. When a function is defined by a formula, then any given interval of integration can be partitioned in such a way that Simpson's rule can be applied. Several examples have demonstrated that for N = 8, accuracy to 4 decimal places

can usually be obtained by Simpson's method. This means that hand computations could suffice if a computer is not available. Because of the preceeding observations, it should not be surprising that Simpson's rule is widely used in practical computations.

BIBLIOGRAPHY

The following abbreviations are used:
AMM - American Mathematical Monthly
MT - Mathematics Teacher

Arden, B. and K. Astill, Numerical Algorithms: Origins and Applications, Addison-Wesley, Reading, MA, 1970.

Beckett, R. and J. Hurt, Numerical Calculations and Algorithms, McGraw-Hill Book Company, New York, 1967.

Dorn, W.S., G.G. Bitter, and D.L. Hector, Computer Applications For Calculus, Prindle, Weber and Schmidt, Inc., Boston, 1972.

Ellis, R. and D. Gulick, Calculus with Analytic Geometry, Harcourt Brace Jovanovich, Inc., New York, 1978.

Flanders, H., R. Korfhage, and J. Price, Calculus, Academic Press, Inc., New York, 1970.

Forsythe, G.E., "Pit Falls in Computation, or Why a Math Book Isn't Enough," AMM 77 (1970), 931-956.

Gear, C.W., Applications and Algorithms in Science and Engineering, Science Research Associates, Inc., Chicago, 1978.

Henriksen, M. and M. Lees, Single Variable Calculus, Worth Publishers, Inc., New York, 1970.

Kemeny, J.G. and T.E. Kurtz, BASIC Programming, Second Edition, John Wiley and Sons, Inc., New York, 1971.

Kuller, R.G., "Computer-Oriented Calculus," Proceedings of a Conference on Computers in the Undergraduate Curricula, University of Iowa, Iowa City, 1970, pp. 4.1-4.11.

Leinbach, L.C., Calculus with the Computer, Prentice-Hall, Inc., Englewood Cliffs, N.J., 1974.

Lynch, R. and D. Ostberg, Calculus with Computer Applications, Xerox College Publishing, Lexington, MA, 1973.

McAloon, K. and A. Tromba, Calculus (Volume 1BCD), Harcourt Brace Jovanovich, Inc., New York, 1972.

McCracken, D. and W. Dorn, Numerical Methods and Fortran Programming, John Wiley and Sons, Inc., New York, 1964.

Monzino, M.G., "On Simpson's Rule," MT 67 (1974), p. 165.

Moursund, D. and C. Duris, Elementary Theory and Application of Numerical Analysis, McGraw-Hill, New York, 1967.

Peters, G.O. and C.E. Mailey, "Numerical Integration Over Any Number of Equal Intervals," AMM 75 (1968), pp. 741-744.

Protter, M. and C. Morrey, Jr., College Calculus with Analytic Geometry, Third Edition, Addison-Wesley Publishing Company, Reading, MA, 1977.

Ralston, A., A First Course in Numerical Analysis, McGraw-Hill, New York, 1965.

Shenk, A., Calculus and Analytic Geometry, Goodyear Publishing Company, Santa Monica, CA, 1977.

Smith, D.A., INTERFACE: Calculus and the Computer, Houghton Mifflin Company, Boston, MA, 1976.

Thesing, G.L. and C.A. Wood, "Using the Computer as a Discovery Tool in Calculus," AMM 81 (1974), pp. 163-168.

APPENDIX A

Mathematical Functions

The following are standard mathematical functions which can be referenced by the BASIC program. In these functions, (ne) can be a numeric expression of any complexity and may include other function references. The quantity (ne) is an argument (parameter) of the function.

FUNCTION	DECSRIPTION
ABS(ne)	Finds the absolute value of ne.
ATN(ne)	Finds the arctangent of ne in the principal value range $-\pi/2$ to $+\pi/2$.
COS(ne)	Finds the cosine of ne; the angle ne is expressed in radians.
EXP(ne)	Finds the value of e to the power of ne.
INT(ne)	Finds the largest integer not greater than ne. Example: INT(5.95) = 5 and INT(-5.95) = -6.
LGT(ne)	Finds the base 10 logarithm of ne; ne > 0, otherwise an execution error causes program termination.
LOG(ne)	Finds the natural logarithm of ne; ne > 0, otherwise an execution error causes program termination.
SIN(ne)	Finds the sine of ne; the angle ne is expressed in radians.
SQR(ne)	Finds the square root of ne; ne > 0, otherwise an execution error causes program termination.
TAN(ne)	Finds the tangent of ne; the angle ne is expressed in radians.

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APPENDIX B

Suppose we want to approximate the curve of $F(x) = 1/1+x^2$ by a quadratic function $g(x) = ax^2 + bx + c$ over the interval [0,1]. We must use three points on the graph of F(x) say (0,1), (1,4/5), and (1,1/2). These choices make use of the partition [0,1/2], [1/2,1] of the interval [0,1]. Since g(0) = F(0), g(1/2) = F(1/2), and g(1) = F(1) we have the system of 3 equations with 3 unknowns a, b, c as follows:

$$a\cdot 0^2 + b\cdot 0 + c = 1 \qquad c = 1$$

$$a(1/2)^2 + b(1/2) + c = 4/5 \qquad a\cdot 1/4 + b\cdot 1/2 + c = 4/5$$

$$a(1)^2 + b(1) + c = 1/2 \qquad a\cdot 1 + b\cdot 1 + c = 1/2$$

This simplifies to

$$c = 1$$

$$5a + 10b + 20c = 16$$

$$2a + 2b + 2c = 1$$

The solutions are c = 1, a = -1/5, and b = -3/10 so that

$$g(x) = \frac{-x^2}{5} - \frac{3x}{10} + 1.$$

Observe that

$$\int_0^1 g(x)\,dx = \frac{47}{60}$$

and Formula (4-b) of Simpson's approximation gives

$$\int_0^1 F(x)\,dx = \frac{1}{3}\cdot\frac{1}{2}(F(0) + 4F(1/2) + F(1)) = \frac{47}{60}$$

also when the subdivision $0 = x_0$, $1/2 = x_1$, $1 = x_2$ of [0,1] is used.

The above procedure is often called the method of undetermined coefficients. If we had 4 points of some function, say (-1,1/2), (0,1), (1,2), (2,4), we could

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approximate this by a third degree polynomial $p(x) = ax^3 + bx^2 + cx + d$. The equations $p(-1) = 1/2$, $p(0) = 1$, $p(1) = 2$, and $p(2) = 4$ translate into

$$\begin{aligned} -a + b - c + d &= 1/2 \\ d &= 1 \\ a + b + c + d &= 2 \\ 8a + 4b + 2c + d &= 4. \end{aligned}$$

After some labor, one finds $a = 1/12$, $b = 1/4$, $c = 2/3$, $d = 1$, and

$$p(x) = \frac{x^3}{12} + \frac{x^2}{4} + \frac{2x}{3} + 1.$$

In general, to approximate a function by a polynomial of degree n, i.e.,

$$p(x) = a_n x^x + a_{n-1}x^{n-1} + \ldots + a_1 x + a_0$$

requires (n+1) points on the graph of F(x). These will give n+1 linear equations involving the n+1 unknowns a_n, a_{n-1}, a_{n-2}, ..., a_0. As the above examples illustrate, the method of undetermined coefficients can become quite tedious. A simpler method called Lagrange Interpolation has been devised. A good discussion of this may be found in Flanders (5, p.377-379).

STUDENT FORM 1

Request for Help

Return to:
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Student: If you have trouble with a specific part of this unit, please fill out this form and take it to your instructor for assistance. The information you give will help the author to revise the unit.

Your Name ____________________ Unit No. ______

Page ______ ○ Upper ○ Middle ○ Lower	OR	Section ______ Paragraph ______	OR	Model Exam Problem No. ______ Text Problem No. ______

Description of Difficulty: (Please be specific)

Instructor: Please indicate your resolution of the difficulty in this box.

○ Corrected errors in materials. List corrections here:

○ Gave student better explanation, example, or procedure than in unit. Give brief outline of your addition here:

○ Assisted student in acquiring general learning and problem-solving skills (not using examples from this unit.)

Instructor's Signature ____________________

Please use reverse if necessary.

STUDENT FORM 2

Unit Questionnaire

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Name____________________ Unit No.__________ Date__________

Institution____________________ Course No.__________

Check the choice for each question that comes closest to your personal opinion.

1. How useful was the amount of detail in the unit?

____Not enough detail to understand the unit
____Unit would have been clearer with more detail
____Appropriate amount of detail
____Unit was occasionally too detailed, but this was not distracting
____Too much detail; I was often distracted

2. How helpful were the problem answers?

____Sample solutions were too brief; I could not do the intermediate steps
____Sufficient information was given to solve the problems
____Sample solutions were too detailed; I didn't need them

3. Except for fulfilling the prerequisites, how much did you use other sources (for example, instructor, friends, or other books) in order to understand the unit?

____A Lot ____Somewhat ____A Little ____Not at all

4. How long was this unit in comparison to the amount of time you generally spend on a lesson (lecture and homework assignment) in a typical math or science course?

____Much Longer ____Somewhat Longer ____About the Same ____Somewhat Shorter ____Much Shorter

5. Were any of the following parts of the unit confusing or distracting? (Check as many as apply.)

____Prerequisites
____Statement of skills and concepts (objectives)
____Paragraph headings
____Examples
____Special Assistance Supplement (if present)
____Other, please explain____________________

6. Were any of the following parts of the unit particularly helpful? (Check as many as apply.)

____Prerequisites
____Statement of skills and concepts (objectives)
____Examples
____Problems
____Paragraph headings
____Table of Contents
____Special Assistance Supplement (if present)
____Other, please explain____________________

Please describe anything in the unit that you did not particularly like.

Please describe anything that you found particularly helpful. (Please use the back of this sheet if you need more space.)