ELEMENTARY NUMERICAL ANALYSIS

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PREFACE

This book gives an introduction to numerical analysis, and it is intended for use by undergraduates in the sciences, mathematics, and engineering. The main prerequisite for using the book is a one-year course in the calculus of functions of one variable; some knowledge of computer programming is also needed. With this background, the book can be used for a sophomore-level course in numerical analysis. The last two chapters of the textbook are on numerical methods for linear algebra and ordinary differential equations. A background in these subjects would be helpful, but these chapters include the necessary theoretical material.

Students taking a course in numerical analysis do so for a variety of reasons. Some will need it in other subjects, in research, or in their careers. Others will be taking it to broaden their knowledge of computing. When I teach this course, I have several objectives for the students. First, they should obtain an intuitive and working understanding of some numerical methods for the basic problems of numerical analysis (as specified by the chapter headings). Second, they should gain some appreciation of the concept of error and of the need to analyze and predict it. And third, they should develop some experience in the implementation of numerical methods using a computer. This should include an appreciation of computer arithmetic and its effects.

The book covers most of the standard topics in a numerical analysis course, and it also explores some of the main underlying themes of the subject. Among these are the approximation of problems by simpler problems, the construction of algorithms, iteration methods, error analysis, stability, asymptotic error formulas, and the effects of machine arithmetic. Because of the level of the course, emphasis has been placed on obtaining an intuitive understanding of both the problem at hand and the numerical methods being used to solve it. The examples have been carefully chosen to develop this understanding, not just to illustrate an algorithm. Proofs are included only where they are sufficiently simple and where they add to an intuitive understanding of the result.

For the introduction to computer programming, the preferred language in the world of scientific computing is Fortran. In this text I have used Fortran 77, the new Fortran standard. It permits much better programming practices, and the programs written in it are much easier to understand than those written in Fortran 66. I have found that students experienced in Pascal can learn Fortran 77 very rapidly during the course.

The Fortran programs are included for several reasons. First, they illustrate the construction of algorithms. Second, they save the students from having to write as many programs, allowing them to spend more time on experimentally learning about a numerical method. After all, the main focus of the course should be numerical analysis, not learning how to program. Third, the programs provide examples of the language Fortran 77 and of good programming practices using it. Of course, the students should write some programs of their own. Some of these can be simple modifications of the included programs, for example, modifying the Simpson integration code to one for the trapezoidal rule. Other programs should be more substantial and original. The Fortran 77 programs of this text are available on a floppy disk, included with the instructor's manual for the text.

There are exercises at the end of each section in the book. These are of several types. Some exercises provide additional illustrations of the theoretical results given in the section, and many of these can be done with either a hand calculator or with a simple computer program. Other exercises are to further explore the theoretical material of the section, perhaps developing some additional theoretical results. In some sections, exercises are given that require more substantial programs; many of these exercises can be done in conjunction with package programs such as those discussed in Appendix C.

In teaching a one-semester course from this textbook, I cover the material in the order given here. The material can be taught in some other order, but I suggest that Chapters 1 through 3 be covered first. Following that, Chapter 8 on linear algebra can be included at any point. The material on polynomial interpolation in Chapter 5 will be needed before covering Chapters 6, 7, and 9. The textbook contains more than enough material for a one-semester course, and the instructor has considerable leeway in what to leave out.

I would like to thank my colleagues Dan Anderson, Herb Hethcote, and Keith Stroyan of the University of Iowa for their comments on the text. I also thank the reviewers of the manuscript for their suggestions, which were very helpful in preparing the final version of the book. I would like to thank Lois Friday for having done an excellent job of typing the book. Several classes of students have used preliminary versions of this text, and I thank them for their forbearance and suggestions. The staff of John Wiley have been very supportive and helpful in this project, and the text is much better as a result of their efforts, for which

I am grateful. Finally, I would like to thank my wife, Alice, for her patience and support, something that is much needed in a project such as this.

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Iowa City, Iowa
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CONTENTS

ONE

TAYLOR POLYNOMIALS

Numerical analysis uses results and methods from many other areas of mathematics, particularly calculus and linear algebra. In this chapter we consider one of the most useful tools from calculus, Taylor's theorem. This will be needed for both the development and understanding of most of the numerical methods taken up in this text.

The first section introduces Taylor polynomials as a way to evaluate other functions approximately; and the second section gives a precise formula, Taylor's theorem, for the error in these polynomial approximations. The final section discusses the evaluation of polynomials.

Other material from calculus is given in the appendixes. Appendix A contains a complete review of mean-value theorems and Appendix B reviews other results from calculus, algebra, geometry, and trigonometry.

1.1 THE TAYLOR POLYNOMIAL

Most functions $f(x)$ that occur in mathematics cannot be evaluated exactly in any simple way. For example, consider evaluating $f(x) = \cos(x)$, e^x, or $\sqrt{x}$, without using a calculator or computer. To evaluate such expressions, we use functions $\hat{f}(x)$ which are almost equal to $f(x)$ and are easier to evaluate. The most common class of approximating functions $\hat{f}(x)$ are the polynomials. They are easy to work with and they are usually an efficient means of approximating $f(x)$. Among polynomials, the most widely used is the Taylor polynomial. There are other more efficient approximating polynomials, and we study some of them in Chapter 6. But the Taylor polynomial is comparatively easy to construct, and it is often a first step in obtaining more efficient approximations. The Taylor polynomial is also important in several other areas of mathematics.

Let $f(x)$ denote a given function, for example, e^x or $\log(x)$. The Taylor polynomial is constructed to mimic the behavior of $f(x)$ at some point $x = a$. As a result, it will be nearly equal to $f(x)$ at points x near to a. To be more specific, find a linear polynomial $p_1(x)$ for which

$$\begin{aligned} p_1(a) &= f(a) \\ p_1'(a) &= f'(a) \end{aligned} \tag{1.1}$$

Then it is easy to verify that the polynomial is uniquely given by

$$p_1(x) = f(a) + (x - a)f'(a) \tag{1.2}$$

The graph of $y = p_1(x)$ is tangent to that of $y = f(x)$ at $x = a$.

Example

Let $f(x) = e^x$ and $a = 0$. Then

$$p_1(x) = 1 + x$$

The graphs of f and p_1 are given in Figure 1.1. Note that $p_1(x)$ is approximately e^x when x is near 0.

To continue the construction process, consider finding a quadratic polynomial $p_2(x)$ that approximates $f(x)$ at $x = a$. Since there are three coefficients in the formula of a quadratic polynomial,

$$p_2(x) = b_0 + b_1x + b_2x^2$$

it is natural to impose three conditions on $p_2(x)$ in order to determine

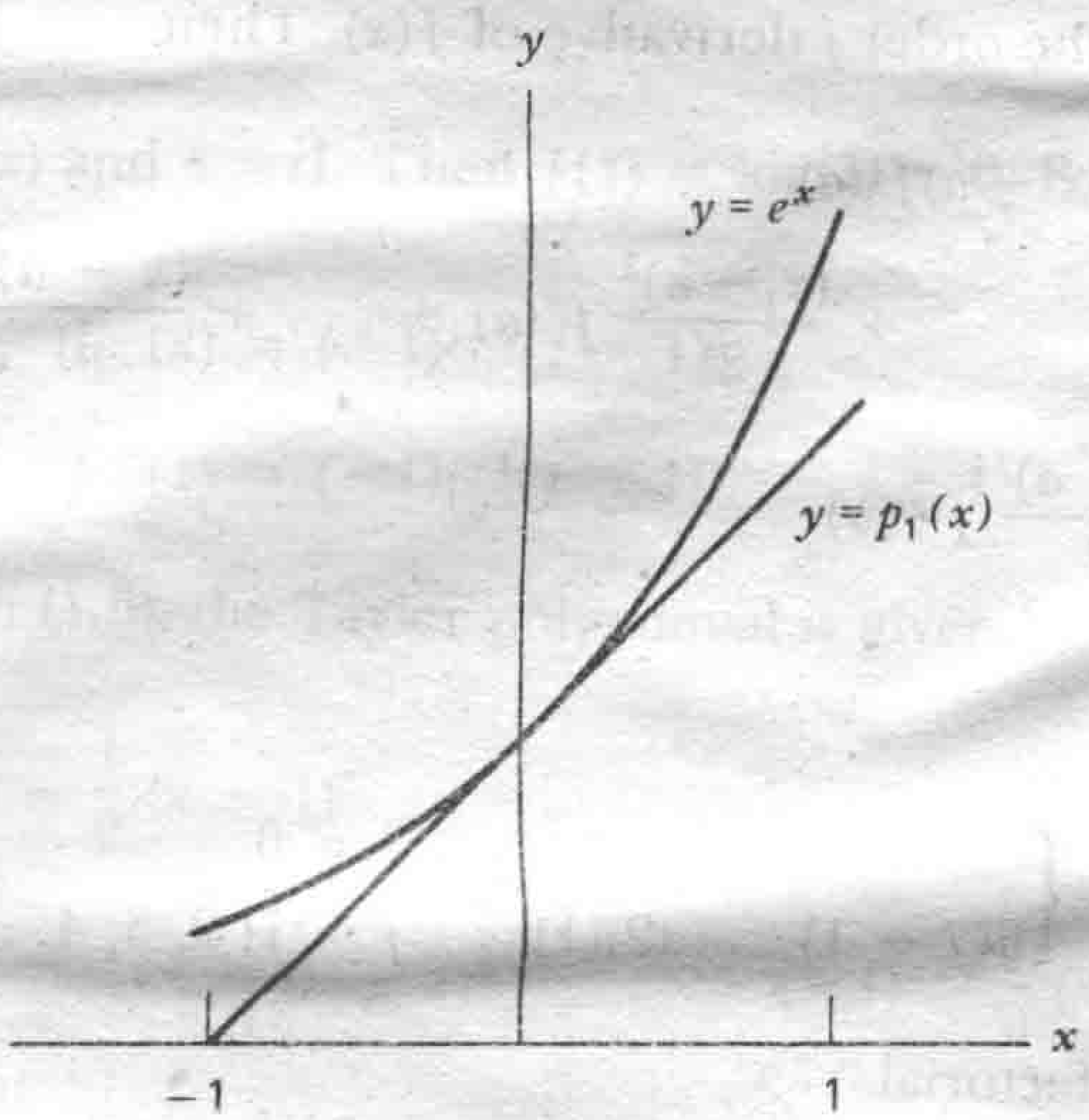

Figure 1.1 $e^x \approx 1 + x$.

them. To better mimic the behavior of $f(x)$ at $x = a$, we require

$$\begin{aligned} p_2(a) &= f(a) \\ p_2'(a) &= f'(a) \\ p_2''(a) &= f''(a) \end{aligned} \tag{1.3}$$

It can be checked that these are satisfied by the formula

$$p_2(x) = f(a) + (x - a)f'(a) + \frac{1}{2}(x - a)^2 f''(a) \tag{1.4}$$

Example

Continuing the previous example of $f(x) = e^x$, we have

$$p_2(x) = 1 + x + \frac{1}{2}x^2$$

We can continue this process of mimicking the behavior of $f(x)$ at $x = a$. Let $p_n(x)$ be a polynomial of degree n, and require it to satisfy

$$p_n^{(j)}(a) = f^{(j)}(a), \qquad j = 0, 1, \ldots, n \tag{1.5}$$

where $f^{(j)}(x)$ is the order j derivative of $f(x)$. Then

$$p_n(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \dots + \frac{(x-a)^n}{n!}f^{(n)}(a) \quad (1.6)$$

$$= \sum_{j=0}^{n} \frac{(x-a)^j}{j!} f^{(j)}(a)$$

In the formula,

$$j! = \begin{cases} 1, & j = 0 \\ j(j-1)\dots(2)(1), & j = 1, 2, 3, 4, \dots \end{cases}$$

and is called "j factorial."

Example

Again let $f(x) = e^x$ and $a = 0$. Then

$$f^{(j)}(x) = e^x, \qquad f^{(j)}(0) = 1, \qquad \text{for all} \qquad j \geqq 0$$

Thus

$$p_n(x) = 1 + x + \frac{1}{2!}x^2 + \dots + \frac{1}{n!}x^n = \sum_{j=0}^{n} \frac{x^j}{j!} \quad (1.7)$$

Table 1.1 contains values of $p_1(x)$, $p_2(x)$, $p_3(x)$, and e^x at various values of x in $[-1, 1]$. For a fixed x, the accuracy improves as the degree n increases. And for a polynomial of fixed degree, the accuracy decreases as x moves away from $a = 0$.

Table 1.1 Taylor Approximations to e^x

x	$p_1(x)$	$p_2(x)$	$p_3(x)$	e^x
−1.0	0	0.500	0.33333	0.36788
−0.5	0.5	0.625	0.60417	0.60653
−0.1	0.9	0.905	0.90483	0.90484
0	1.0	1.000	1.00000	1.00000
0.1	1.1	1.105	1.10517	1.10517
0.5	1.5	1.625	1.64583	1.64872
1.0	2.0	2.500	2.66667	2.71828

Example

Let $f(x) = \log(x)$ and $a = 1$. Then $f(1) = \log(1) = 0$. By induction,

$$f^{(j)}(x) = (-1)^{j-1}(j-1)!\,\frac{1}{x^j}$$

$$f^{(j)}(1) = (-1)^{j-1}(j-1)!, \qquad j \geqq 1$$

If this is used in (1.6), the Taylor polynomial is given by

$$p_n(x) = (x-1) - \frac{1}{2}(x-1)^2 + \frac{1}{3}(x-1)^3 - \cdots + (-1)^{n-1}\frac{1}{n}(x-1)^n \qquad (1.8)$$

$$= \sum_{j=1}^{n} \frac{(-1)^{j-1}}{j}(x-1)^j$$

PROBLEMS

1. Using (1.8), compare $\log(x)$ and its Taylor polynomials of degrees 1, 2, and 3, in the manner of Table 1.1. Do this on the interval $[\frac{1}{2}, \frac{3}{2}]$.
2. Produce the linear and quadratic Taylor polynomials for the following cases.
   (a) $f(x) = \sqrt{x}$, $a = 1$
   (b) $f(x) = \sin(x)$, $a = \pi/4$
   (c) $f(x) = e^{\cos(x)}$, $a = 0$
3. Produce a general formula for the degree n Taylor polynomials for the following functions, all using $a = 0$ as the point of approximation.
   (a) $1/(1-x)$
   (b) $\sin(x)$
   (c) $\sqrt{1+x}$
4. Compare $f(x) = \sin(x)$ with its Taylor polynomials of degrees 1, 3, and 5, on the interval $-\pi/2 \leqq x \leqq \pi/2$; $a = 0$. Produce a table in the manner of Table 1.1.
5. (a) Produce the Taylor polynomials of degrees 1, 2, 3, and 4 for $f(x) = e^{-x}$, with $a = 0$ the point of approximation.
   (b) Using the Taylor polynomials for e^t, substitute $t = -x$ to obtain polynomial approximations for e^{-x}. Compare with (a).

6. Repeat problem 5 with $f(x) = e^{x^2}$.
7. The quotient

$$g(x) = \frac{e^x - 1}{x}$$

is undefined for $x = 0$. Approximate e^x using Taylor polynomials of degrees 1, 2, and 3, in turn, to determine a natural definition of $g(0)$.

8. Repeat problem 7 with $g(x) = (1/x) \log (1 + x)$.
9. (a) As an alternative to the linear Taylor polynomial, construct a linear polynomial $q(x)$, satisfying

$$q(a) = f(a), \qquad q(b) = f(b)$$

for given points a and b.

(b) Apply this to $f(x) = e^x$ with $a = 0$ and $b = 1$. For $0 \leqq x \leqq 1$, numerically compare $q(x)$ with the linear Taylor polynomial of this section.

10. For $f(x) = e^x$, construct a cubic polynomial $q(x)$ for which

$$q(0) = f(0), \qquad q(1) = f(1)$$
$$q'(0) = f'(0), \qquad q'(1) = f'(1)$$

Compare it to e^x and the Taylor polynomial $p_3(x)$ of (1.6).
Hint: Write $q(x) = b_0 + b_1x + b_2x^2 + b_3x^3$. Determine b_0 and b_1 from the conditions at $x = 0$. Then obtain a linear system of two equations for the remaining coefficients b_2 and b_3.

1.2 THE ERROR IN TAYLOR'S POLYNOMIAL

To make practical use of the Taylor polynomial approximation to $f(x)$, we need to know its accuracy. The following theorem gives the main way of estimating this accuracy. We present it without proof, since it is given in most calculus texts.

Theorem 1.1 (Taylor's Theorem)

Assume that $f(x)$ has $n + 1$ continuous derivatives on an interval $\alpha \leqq x \leqq \beta$, and let the point a belong to that interval. For the Taylor polynomial $p_n(x)$ of (1.6), let $R_n(x) \equiv f(x) - p_n(x)$ denote the remainder in approximating $f(x)$ by $p_n(x)$. Then,

$$R_n(x) = \frac{(x-a)^{n+1}}{(n+1)!} f^{(n+1)}(c_x), \qquad \alpha \leqq x \leqq \beta \tag{1.9}$$

with c_x an unknown point between a and x.

Example

Let $f(x) = e^x$ and $a = 0$. The Taylor polynomial is given in (1.7). From the above theorem, the approximation error is given by

$$e^x - p_n(x) = \frac{x^{n+1}}{(n+1)!} e^c, \qquad n \geqq 0 \tag{1.10}$$

with c between 0 and x.

As a special case, take $x = 1$. Then from (1.7),

$$e \approx p_n(1) = 1 + 1 + \frac{1}{2!} + \frac{1}{3!} + \ldots + \frac{1}{n!}$$

and from (1.10),

$$e - p_n(1) = R_n(1) = \frac{e^c}{(n+1)!}, \qquad 0 < c < 1$$

From definitions of e given in most calculus texts, it is easy to obtain a bound of $e < 3$. Thus we can bound $R_n(1)$:

$$\frac{1}{(n+1)!} \leqq R_n(1) \leqq \frac{e}{(n+1)!} < \frac{3}{(n+1)!}$$

This uses the inequality $e^0 \leqq e^c \leqq e^1$. As an actual numerical example, suppose we want to approximate e by $p_n(1)$ with

$$R_n(1) \leqq 10^{-9}$$

Since we only know an upper bound for $R_n(1)$, we can obtain the desired error by making the upper bound satisfy

$$\frac{3}{(n+1)!} \leqq 10^{-9}$$

This is true when $n \geqq 12$; thus $p_{12}(1)$ is a sufficiently accurate approximation to e.

The formulas (1.6) and (1.9) can be used to form approximations and remainder formulas for most of the standard functions encountered in undergraduate mathematics. For later reference, we give some of the more important ones.

$$e^x = 1 + x + \frac{x^2}{2!} + \cdots + \frac{x^n}{n!} + \frac{x^{n+1}}{(n+1)!} e^c \qquad (1.11)$$

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots + (-1)^{n-1} \frac{x^{2n-1}}{(2n-1)!} + (-1)^n \frac{x^{2n+1}}{(2n+1)!} \cos(c) \qquad (1.12)$$

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots + (-1)^n \frac{x^{2n}}{(2n)!} + (-1)^{n+1} \frac{x^{2n+2}}{(2n+2)!} \cos(c) \qquad (1.13)$$

$$\frac{1}{1-x} = 1 + x + x^2 + \cdots + x^n + \frac{x^{n+1}}{1-x}, \qquad x \neq 1 \qquad (1.14)$$

$$(1+x)^\alpha = 1 + \binom{\alpha}{1} x + \binom{\alpha}{2} x^2 + \cdots + \binom{\alpha}{n} x^n + \binom{\alpha}{n+1} x^{n+1} (1+c)^{\alpha-n-1} \qquad (1.15)$$

In this last formula, α is any real number. The coefficients $\binom{\alpha}{k}$ are called binomial coefficients and are defined by

$$\binom{\alpha}{k} = \frac{\alpha(\alpha-1)\cdots(\alpha-k+1)}{k!}, \qquad k = 1, 2, 3, \ldots$$

In all of the formulas, except (1.14), the point c is between 0 and x.

By rearranging the terms in (1.14), we obtain the sum of a finite geometric series or progression,

$$1 + x + x^2 + \cdots + x^n = \frac{1 - x^{n+1}}{1-x}, \qquad x \neq 1 \qquad (1.16)$$

And by letting $n \to \infty$ in (1.14) when $|x| < 1$, we obtain the infinite *geometric series*

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 + \ldots = \sum_{j=0}^{\infty} x^j, \qquad |x| < 1 \qquad (1.17)$$

Example

Approximate cos(x) for $|x| \leqq \pi/4$, with an error of no greater than 10^{-5}. Since the point c in the remainder of (1.13) is unknown, we consider the worst possible case and make it satisfy the desired error bound:

$$|R_{2n+1}(x)| \leqq \frac{x^{2n+2}}{(2n+2)!} \leqq 10^{-5}, \qquad \text{for } |x| \leqq \pi/4$$

This uses $|\cos(c)| \leqq 1$. For this inequality to be true, we must have

$$\frac{(\pi/4)^{2n+2}}{(2n+2)!} \leqq 10^{-5}$$

which is satisfied when $n \geqq 3$. The desired approximation is

$$\cos(x) \approx 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!}$$

Not all Taylor polynomials or remainder terms are created directly from (1.6) and (1.9). Rather, the above standard series are manipulated. For example, to obtain a series for $\log(1-t)$, integrate (1.14). More precisely,

$$\int_0^t \frac{dx}{1-x} = \int_0^t (1 + x + x^2 + \ldots + x^n)\, dx + \int_0^t \frac{x^{n+1}}{1-x}\, dx$$

$$-\log(1-t) = t + \frac{1}{2}t^2 + \frac{1}{3}t^3 + \ldots + \frac{1}{n+1}t^{n+1} + \int_0^t \frac{x^{n+1}}{1-x}\, dx$$

$$\log(1-t) = -\left(t + \frac{1}{2}t^2 + \ldots + \frac{1}{n+1}t^{n+1}\right) - \int_0^t \frac{x^{n+1}}{1-x}\, dx \qquad (1.18)$$

This is valid for $t < 1$. The remainder term can be simplified by applying