6

Polynomial interpolation

6.1 Introduction

It is time to take a break from solving equations. In this chapter we consider the problem of polynomial interpolation; it involves finding a polynomial that agrees exactly with some information that we have about a real-valued function f of a single real variable x. This information may be in the form of values $f(x_0), \dots, f(x_n)$ of the function f at some finite set of points $\{x_0, \dots, x_n\}$ on the real line, and the corresponding polynomial is then called the **Lagrange interpolation polynomial**[1] or, provided that f is differentiable, it may include values of the derivative of f at these points, in which case the associated polynomial is referred to as a **Hermite interpolation polynomial**.[2]

Why should we be interested in constructing Lagrange or Hermite interpolation polynomials? If the function values $f(x)$ are known for all x in a closed interval of the real line, then the aim of polynomial

[1] Joseph-Louis Lagrange (25 January 1736, Turin, Sardinia–Piedmont (now in Italy) – 10 April 1813, Paris, France) made fundamental contributions to the calculus of variations. He succeeded Euler as Director of Mathematics at the Berlin Academy of Sciences in 1766. During his stay in Berlin Lagrange worked on astronomy, the stability of the solar system, mechanics, dynamics, fluid mechanics, probability, number theory, and the foundations of calculus. In 1787 he moved to Paris and became a member of the Académie des Sciences. Napoleon named Lagrange to the Legion of Honour and as a Count of the Empire in 1808, and on 3 April 1813, a week before his death, he received the Grand Croix of the Ordre Impérial de la Réunion.

[2] Charles Hermite (24 December 1822, Dieuze, Lorraine, France – 14 January 1901, Paris, France). Hermite did not enjoy formal examinations and had to spend five years to complete his undergraduate degree. He contributed to the theory of elliptic functions and their application to the general polynomial equation of the fifth degree. In 1873 he published the first proof that e is a transcendental number. Using methods similar to those of Hermite, Lindemann established in 1882 that π was also transcendental. A number of mathematical entities bear Hermite's name: Hermite orthogonal polynomials, Hermite's differential equation, Hermite's formula of interpolation and Hermitian matrices.

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interpolation is to approximate the function f by a polynomial over this interval. Given that any polynomial can be completely specified by its (finitely many) coefficients, storing the interpolation polynomial for f in a computer will be, generally, more economical than storing f itself.

Frequently, it is the case, though, that the function values $f(x)$ are only known at a finite set of points $x_0, \dots, x_n$, perhaps as the results of some measurements. The aim of polynomial interpolation is then to attempt to reconstruct the unknown function f by seeking a polynomial p_n whose graph in the (x, y)-plane passes through the points with coordinates $(x_i, f(x_i))$, $i = 0, \dots, n$. Of course, in general, the resulting polynomial p_n will differ from f (unless f itself is a polynomial of the same degree as p_n), so an error will be incurred. In this chapter we shall also establish results which provide bounds on the size of this error.

6.2 Lagrange interpolation

Given that n is a nonnegative integer, let $\mathcal{P}_n$ denote the set of all (real-valued) polynomials of degree $\le n$ defined over the set $\mathbb{R}$ of real numbers. The simplest interpolation problem can be stated as follows: given x_0 and y_0 in $\mathbb{R}$, find a polynomial $p_0 \in \mathcal{P}_0$ such that $p_0(x_0) = y_0$. The solution to this is, trivially, $p_0(x) \equiv y_0$. The purpose of this section is to explore the following more general problem.

> Let $n \ge 1$, and suppose that $x_i, i = 0, 1, \dots, n$, are *distinct* real numbers (*i.e.*, $x_i \ne x_j$ for $i \ne j$) and $y_i, i = 0, 1, \dots, n$, are real numbers; we wish to find $p_n \in \mathcal{P}_n$ such that $p_n(x_i) = y_i$, $i = 0, 1, \dots, n$.

To prove that this problem has a unique solution, we begin with a useful lemma.

Lemma 6.1 *Suppose that $n \ge 1$. There exist polynomials $L_k \in \mathcal{P}_n$, $k = 0, 1, \dots, n$, such that*

$$L_k(x_i) = \begin{cases} 1\,, & i = k\,, \\ 0\,, & i \ne k\,, \end{cases} \tag{6.1}$$

for all $i, k = 0, 1, \dots, n$. Moreover,

$$p_n(x) = \sum_{k=0}^{n} L_k(x) y_k \tag{6.2}$$

satisfies the above interpolation conditions; in other words, $p_n \in \mathcal{P}_n$ and $p_n(x_i) = y_i$, $i = 0, 1, \dots, n$.

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Proof For each fixed k, $0 \le k \le n$, L_k is required to have n zeros – x_i, $i = 0, 1, \ldots, n$, $i \ne k$; thus, $L_k(x)$ is of the form

$$L_k(x) = C_k \prod_{\substack{i=0\\ i\ne k}}^{n} (x - x_i)\,, \tag{6.3}$$

where $C_k \in \mathbb{R}$ is a constant to be determined. It is easy to find the value of C_k by recalling that $L_k(x_k) = 1$; using this in (6.3) yields

$$C_k = \prod_{\substack{i=0\\ i\ne k}}^{n} \frac{1}{x_k - x_i}\,.$$

On inserting this expression for C_k into (6.3) we get

$$L_k(x) = \prod_{\substack{i=0\\ i\ne k}}^{n} \frac{x - x_i}{x_k - x_i}\,. \tag{6.4}$$

As the function p_n defined by (6.2) is a linear combination of the polynomials $L_k \in \mathcal{P}_n$, $k = 0, 1, \ldots, n$, also $p_n \in \mathcal{P}_n$. Finally, $p_n(x_i) = y_i$ for $i = 0, 1, \ldots, n$ is a trivial consequence of using (6.1) in (6.2). $\square$

Remark 6.1 *Although the statement of Lemma 6.1 required that $n \ge 1$, the trivial case of $n = 0$ mentioned at the beginning of the section can also be included by defining, for $n = 0$, $L_0(x) \equiv 1$, and observing that the function p_0 defined by*

$$p_0(x) = L_0(x)y_0 \ (\equiv y_0\,)$$

is the unique polynomial in $\mathcal{P}_0$ that satisfies $p_0(x_0) = y_0$.

We note that, implicitly, the polynomials L_k, $k = 0, 1, \ldots, n$, depend on the polynomial degree n, $n \ge 0$. To highlight this fact, a more accurate but cumbersome notation would have involved writing, for example, $L_k^n(x)$ instead of $L_k(x)$; this would have made it clear that $L_k^n(x)$ differs from $L_k^m(x)$ when the polynomial degrees n and m differ. For the sake of notational simplicity, we have chosen to write $L_k(x)$; the implied value of n will always be clear from the context.

Theorem 6.1 (Lagrange's Interpolation Theorem) *Assume that $n \ge 0$. Let x_i, $i = 0, \ldots, n$, be* distinct *real numbers and suppose that $y_i, i = 0, \ldots, n$, are real numbers. Then, there exists a unique polynomial $p_n \in \mathcal{P}_n$ such that*

$$p_n(x_i) = y_i\,, \quad i = 0, \ldots, n\,. \tag{6.5}$$

Proof In view of Remark 6.1, for $n = 0$ the proof is trivial. Let us therefore suppose that $n \geq 1$. It follows immediately from Lemma 6.1 that the polynomial $p_n \in \mathcal{P}_n$ defined by

$$p_n(x) = \sum_{k=0}^{n} L_k(x) y_k$$

satisfies the conditions (6.5), thus showing the *existence* of the required polynomial. It remains to show that p_n is the *unique* polynomial in $\mathcal{P}_n$ satisfying the interpolation property

$$p_n(x_i) = y_i\,, \qquad i = 0, 1, \ldots, n\,.$$

Suppose, otherwise, that there exists $q_n \in \mathcal{P}_n$, different from p_n, such that $q_n(x_i) = y_i$, $i = 0, 1, \ldots, n$. Then, $p_n - q_n \in \mathcal{P}_n$ and $p_n - q_n$ has $n+1$ distinct roots, x_i, $i = 0, 1, \ldots, n$; since a polynomial of degree n cannot have more than n distinct roots, unless it is identically 0, it follows that

$$p_n(x) - q_n(x) \equiv 0\,,$$

which contradicts our assumption that p_n and q_n are distinct. Hence, there exists only one polynomial $p_n \in \mathcal{P}_n$ which satisfies (6.5). $\square$

Definition 6.1 *Suppose that $n \geq 0$. Let x_i, $i = 0, \ldots, n$, be distinct real numbers, and y_i, $i = 0, \ldots, n$, real numbers. The polynomial p_n defined by*

$$\boxed{p_n(x) = \sum_{k=0}^{n} L_k(x) y_k\,, \qquad (6.6)}$$

with $L_k(x)$, $k = 0, 1, \ldots, n$, defined by (6.4) when $n \geq 1$, and $L_0(x) \equiv 1$ when $n = 0$, is called the **Lagrange interpolation polynomial** *of degree n for the set of points $\{(x_i, y_i)\colon i = 0, \ldots, n\}$. The numbers x_i, $i = 0, \ldots, n$, are called the* **interpolation points**.

Frequently, the real numbers y_i are given as the values of a real-valued function f, defined on a closed real interval $[a, b]$, at the (distinct) interpolation points $x_i \in [a, b]$, $i = 0, \ldots, n$.

Definition 6.2 *Let $n \geq 0$. Given the real-valued function f, defined and continuous on a closed real interval $[a, b]$, and the (distinct) interpolation points $x_i \in [a, b]$, $i = 0, \ldots, n$, the polynomial p_n defined by*

$$\boxed{p_n(x) = \sum_{k=0}^{n} L_k(x) f(x_k)} \tag{6.7}$$

is the **Lagrange interpolation polynomial of degree** n **(with interpolation points** x_i**,** $i = 0, \dots, n$**) for the function** f*.*

Example 6.1 *We shall construct the Lagrange interpolation polynomial of degree* 2 *for the function* $f\colon x \mapsto \mathrm{e}^x$ *on the interval* $[-1, 1]$*, with interpolation points* $x_0 = -1$*,* $x_1 = 0$*,* $x_2 = 1$*.*

As $n = 2$, we have that

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} = \tfrac{1}{2}x(x-1)\,.$$

Similarly, $L_1(x) = 1 - x^2$ and $L_2(x) = \frac{1}{2}x(x+1)$. Therefore,

$$p_2(x) = \tfrac{1}{2}x(x-1)\,\mathrm{e}^{-1} + (1 - x^2)\,\mathrm{e}^0 + \tfrac{1}{2}x(x+1)\,\mathrm{e}^1\,.$$

Thus, after some simplification, $p_2(x) = 1 + x\sinh 1 + x^2(\cosh 1 - 1)$. ◇

Although the values of the function f and those of its Lagrange interpolation polynomial coincide at the interpolation points, $f(x)$ may be quite different from $p_n(x)$ when x is *not* an interpolation point. Thus, it is natural to ask just how large the difference $f(x) - p_n(x)$ is when $x \neq x_i$, $i = 0, \dots, n$. Assuming that the function f is sufficiently smooth, an estimate of the size of the **interpolation error** $f(x) - p_n(x)$ is given in the next theorem.

Theorem 6.2 *Suppose that* $n \geq 0$*, and that* f *is a real-valued function, defined and continuous on the closed real interval* $[a, b]$*, such that the derivative of* f *of order* $n + 1$ *exists and is continuous on* $[a, b]$*. Then, given that* $x \in [a, b]$*, there exists* $\xi = \xi(x)$ *in* (a, b) *such that*

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\pi_{n+1}(x)\,, \tag{6.8}$$

where

$$\pi_{n+1}(x) = (x - x_0)\dots(x - x_n)\,. \tag{6.9}$$

Moreover

$$|f(x) - p_n(x)| \leq \frac{M_{n+1}}{(n+1)!}|\pi_{n+1}(x)|\,, \tag{6.10}$$

where

$$M_{n+1} = \max_{\zeta\in[a,b]} |f^{(n+1)}(\zeta)|\,.$$

Proof When $x = x_i$ for some i, $i = 0, 1, \dots, n$, both sides of (6.8) are zero, and the equality is trivially satisfied. Suppose then that $x \in [a, b]$ and $x \neq x_i$, $i = 0, 1, \dots, n$. For such a value of x, let us consider the auxiliary function $t \mapsto \varphi(t)$, defined on the interval $[a, b]$ by

$$\varphi(t) = f(t) - p_n(t) - \frac{f(x) - p_n(x)}{\pi_{n+1}(x)}\pi_{n+1}(t)\,. \tag{6.11}$$

Clearly $\varphi(x_i) = 0$, $i = 0, 1, \dots, n$, and $\varphi(x) = 0$. Thus, φ vanishes at $n + 2$ points which are all distinct in $[a, b]$. Consequently, by Rolle's Theorem, Theorem A.2, $\varphi'(t)$, the first derivative of φ with respect to t, vanishes at $n + 1$ points in (a, b), one between each pair of consecutive points at which φ vanishes.

In particular, if $n = 0$, we then deduce the existence of $\xi = \xi(x)$ in the interval (a, b) such that $\varphi'(\xi) = 0$. Since $p_0(x) \equiv f(x_0)$ and $\pi_1(t) = t - x_0$, it follows from (6.11) that

$$0 = \varphi'(\xi) = f'(\xi) - \frac{f(x) - p_0(x)}{\pi_1(x)}\,,$$

and hence (6.8) in the case of $n = 0$.

Now suppose that $n \geq 1$. As $\varphi'(t)$ vanishes at $n+1$ points in (a, b), one between each pair of consecutive points at which φ vanishes, applying Rolle's Theorem again, we see that φ'' vanishes at n distinct points. Our assumptions about f are sufficient to apply Rolle's Theorem $n + 1$ times in succession, showing that $\varphi^{(n+1)}$ vanishes at some point $\xi \in (a, b)$, the exact value of ξ being dependent on the value of x. By differentiating $n + 1$ times the function φ with respect to t, and noting that p_n is a polynomial of degree n or less, it follows that

$$0 = \varphi^{(n+1)}(\xi) = f^{(n+1)}(\xi) - \frac{f(x) - p_n(x)}{\pi_{n+1}(x)}(n + 1)!$$

Hence

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n + 1)!}\pi_{n+1}(x)\,.$$

In order to prove (6.10), we note that as $f^{(n+1)}$ is a continuous function on $[a, b]$ the same is true of $|f^{(n+1)}|$. Therefore, the function $x \mapsto |f^{(n+1)}(x)|$ is bounded on $[a, b]$ and achieves its maximum there; so (6.10) follows from (6.8). $\square$

It is perhaps worth noting that since the location of ξ in the interval $[a, b]$ is unknown (to the extent that the exact dependence of ξ on x is not revealed by the proof of Theorem 6.2), (6.8) is of little practical value; on the other hand, given the function f, an upper bound on the maximum value of $f^{(n+1)}$ over $[a, b]$ is, at least in principle, possible to obtain, and thereby we can provide an upper bound on the size of the interpolation error by means of inequality (6.10).

6.3 Convergence

An important theoretical question is whether or not a sequence (p_n) of interpolation polynomials for a continuous function f converges to f as $n \to \infty$. This question needs to be made more specific, as p_n depends on the distribution of the interpolation points x_j, $j = 0, 1, \dots, n$, not just on the value of n. Suppose, for example, that we agree to choose equally spaced points, with

$$x_j = a + j(b - a)/n\,, \qquad j = 0, 1, \dots, n\,, \quad n \geq 1\,.$$

The question of convergence then clearly depends on the behaviour of M_{n+1} as n increases. In particular, if

$$\lim_{n\to\infty} \frac{M_{n+1}}{(n+1)!} \max_{x\in[a,b]} |\pi_{n+1}(x)| = 0\,,$$

then, by (6.10),

$$\lim_{n\to\infty} \max_{x\in[a,b]} |f(x) - p_n(x)| = 0\,, \tag{6.12}$$

and we say that the sequence of interpolation polynomials (p_n), with equally spaced points on $[a, b]$, converges to f as $n \to \infty$, uniformly on the interval $[a, b]$.

You may now think that if all derivatives of f exist and are continuous on $[a, b]$, then (6.12) will hold. Unfortunately, this is not so, since the sequence

$$\left(M_{n+1} \max_{x\in[a,b]} |\pi_{n+1}(x)| \right)$$

may tend to ∞, as $n \to \infty$, faster than the sequence $(1/(n + 1)!)$ tends to 0.

In order to convince you of the existence of such ‘pathological’ functions, we consider the sequence of Lagrange interpolation polynomials

Table 6.1. *Runge phenomenon: n denotes the degree of the interpolation polynomial p_n to f, with equally spaced points on* $[-5,5]$. 'Max error' *signifies* $\max_{x\in[-5,5]} |f(x) - p_n(x)|$.

Degree n	Max error
2	0.65
4	0.44
6	0.61
8	1.04
10	1.92
12	3.66
14	7.15
16	14.25
18	28.74
20	58.59
22	121.02
24	252.78

p_n, $n = 0, 1, 2, \ldots$, with equally spaced interpolation points on the interval $[-5, 5]$, to

$$f(x) = \frac{1}{1+x^2}\,, \qquad x \in [-5,5]\,.$$

This example is due to Runge,[1] and the characteristic behaviour exhibited by the sequence of interpolation polynomials p_n in Table 6.1 is referred to as the **Runge phenomenon**: Table 6.1 shows the maximum difference between $f(x)$ and $p_n(x)$ for $-5 \le x \le 5$, for values of n from 2 up to 24. The numbers indicate clearly that the maximum error increases exponentially as n increases. Figure 6.1 shows the interpolation polynomial p_{10}, using the equally spaced interpolation points $x_j = -5 + j$, $j = 0, 1, \ldots, 10$. The sizes of the local maxima near ± 5 grow exponentially as the degree n increases.

Note that, in many ways, the function f is well behaved; all its deriva-

[1] Carle David Tolmé Runge (30 August 1856, Bremen, Germany – 3 January 1927, Göttingen, Germany) studied mathematics and physics at the University of Munich. His doctoral dissertation in 1880 was in the area of differential geometry. Gradually, his research interests shifted to more applied topics: he devised a numerical procedure for the solution of algebraic equations where the roots were expressed as infinite series of rational functions of the coefficients, and in 1887 he started to work on the wavelengths of the spectral lines of elements. In 1904 Runge became Professor of Applied Mathematics in Göttingen. He was a fit and active man: on his 70th birthday he entertained his grandchildren by performing handstands. A few months later he suffered a fatal heart attack.

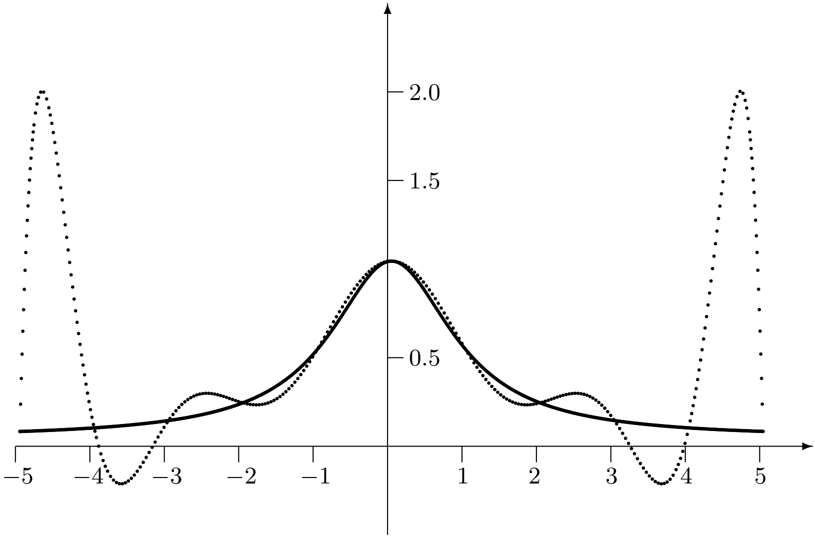

Fig. 6.1. Polynomial interpolation of $f\colon x \mapsto 1/(1+x^2)$ for $x \in [-5,5]$. The continuous curve is f; the dotted curve is the associated Lagrange interpolation polynomial p_{10} of degree 10, using equally spaced interpolation points.

tives are continuous and bounded for all $x \in [-5,5]$. The apparent divergence of the sequence of Lagrange interpolation polynomials (p_n) is related to the fact that, when extended to the complex plane, the Taylor series of the complex-valued function $f\colon z \mapsto 1/(1+z^2)$ converges in the open unit disc of radius 1 but not in any disc of larger radius centred at $z = 0$, given that f has poles on the imaginary axis at $z = \pm\imath$. Some further insight into this problem is given in Exercise 11, and a similar difficulty in numerical integration is discussed in Section 7.4.

6.4 Hermite interpolation

The idea of Lagrange interpolation can be generalised in various ways; we shall consider here one simple extension where a polynomial p is required to take given values and derivative values at the interpolation points. Given the distinct interpolation points $x_i, i = 0,\ldots,n$, and two sets of real numbers y_i, $i = 0,\ldots,n$, and z_i, $i = 0,\ldots,n$, with $n \geq 0$, we need to find a polynomial $p_{2n+1} \in \mathcal{P}_{2n+1}$ such that

$$p_{2n+1}(x_i) = y_i\,, \qquad p'_{2n+1}(x_i) = z_i\,, \qquad i = 0,\ldots,n\,.$$

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The construction is similar to that of the Lagrange interpolation polynomial, but now requires two sets of polynomials H_k and K_k with $k = 0, \ldots, n$; these will be defined in the proof of the next theorem.

Theorem 6.3 (Hermite Interpolation Theorem) *Let $n \geq 0$, and suppose that x_i, $i = 0, \ldots, n$, are* distinct *real numbers. Then, given two sets of real numbers y_i, $i = 0, \ldots, n$, and z_i, $i = 0, \ldots, n$, there is a unique polynomial p_{2n+1} in $\mathcal{P}_{2n+1}$ such that*

$$p_{2n+1}(x_i) = y_i\,, \qquad p'_{2n+1}(x_i) = z_i\,, \qquad i = 0, \ldots, n\,. \tag{6.13}$$

Proof Let us begin by supposing that $n \geq 1$. As in the case of Lagrange interpolation, we start by constructing a set of auxiliary polynomials; we consider the polynomials H_k and K_k, $k = 0, 1, \ldots, n$, defined by

$$\begin{aligned} H_k(x) &= [L_k(x)]^2(1 - 2L'_k(x_k)(x - x_k))\,, \\ K_k(x) &= [L_k(x)]^2(x - x_k)\,, \end{aligned} \tag{6.14}$$

where

$$L_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i}\,.$$

Clearly H_k and K_k, $k = 0, 1, \ldots, n$, are polynomials of degree $2n+1$. It is easy to see that $H_k(x_i) = K_k(x_i) = 0$, $H'_k(x_i) = K'_k(x_i) = 0$ whenever $i, k \in \{0, 1, \ldots, n\}$ and $i \neq k$; moreover, a straightforward calculation verifies their values when $i = k$, showing that

$$\begin{aligned} H_k(x_i) &= \begin{cases} 1\,, & i = k\,, \\ 0\,, & i \neq k\,, \end{cases} \qquad H'_k(x_i) = 0\,, \qquad i, k = 0, 1, \ldots, n\,, \\ K_k(x_i) &= 0\,, \qquad K'_k(x_i) = \begin{cases} 1\,, & i = k\,, \\ 0\,, & i \neq k\,, \end{cases} \qquad i, k = 0, 1, \ldots, n\,. \end{aligned}$$

We deduce that

$$p_{2n+1}(x) = \sum_{k=0}^{n} [H_k(x) y_k + K_k(x) z_k]$$

satisfies the conditions (6.13), and p_{2n+1} is clearly an element of $\mathcal{P}_{2n+1}$.

To show that this is the only polynomial in $\mathcal{P}_{2n+1}$ satisfying these conditions, we suppose otherwise; then, there exists a polynomial q_{2n+1} in $\mathcal{P}_{2n+1}$, distinct from p_{2n+1}, such that

$$q_{2n+1}(x_i) = y_i \quad \text{and} \quad q'_{2n+1}(x_i) = z_i\,, \qquad i = 0, 1, \ldots, n\,.$$

Consequently, $p_{2n+1} - q_{2n+1}$ has $n+1$ distinct zeros; therefore, Rolle's Theorem implies that, in addition to the $n+1$ zeros x_i, $i = 0, 1, \ldots, n$, $p'_{2n+1} - q'_{2n+1}$ vanishes at another n points which interlace the x_i. Hence $p'_{2n+1} - q'_{2n+1} \in \mathcal{P}_{2n}$ has $2n+1$ zeros, which means that $p'_{2n+1} - q'_{2n+1}$ is identically zero, so that $p_{2n+1} - q_{2n+1}$ is a constant function. However, $(p_{2n+1} - q_{2n+1})(x_i) = 0$ for $i = 0, 1, \ldots, n$, and hence $p_{2n+1} - q_{2n+1} \equiv 0$, contradicting the hypothesis that p_{2n+1} and q_{2n+1} are distinct. Thus, p_{2n+1} is unique.

When $n = 0$, we define $H_0(x) \equiv 1$ and $K_0(x) \equiv x - x_0$, which correspond to taking $L_0(x) \equiv 1$ in (6.15). Clearly, p_1 defined by

$$p_1(x) = H_0(x)y_0 + K_0(x)z_0 = y_0 + (x - x_0)z_0$$

is the unique polynomial in $\mathcal{P}_1$ such that $p_1(x_0) = y_0$ and $p'_1(x_0) = z_0$. $\square$

Definition 6.3 *Let $n \geq 0$, and suppose that x_i, $i = 0, \ldots, n$, are distinct real numbers and y_i, z_i, $i = 0, \ldots, n$, are real numbers. The polynomial p_{2n+1} defined by*

$$\boxed{p_{2n+1}(x) = \sum_{k=0}^{n} [H_k(x)y_k + K_k(x)z_k] \qquad (6.15)}$$

where $H_k(x)$ and $K_k(x)$ are defined by (6.15), is called the **Hermite interpolation polynomial** *of degree $2n+1$ for the set of values given in $\{(x_i, y_i, z_i)\colon i = 0, \ldots, n\}$.*

Example 6.2 *We shall construct a cubic polynomial p_3 such that*

$$p_3(0) = 0\,, \quad p_3(1) = 1\,, \quad p'_3(0) = 1 \quad \textit{and} \quad p'_3(1) = 0\,.$$

Here $n = 1$, and since $p_3(0) = p'_3(1) = 0$ the polynomial simplifies to

$$p_3(x) = H_1(x) + K_0(x)\,.$$

We easily find that, with $n = 1$, $x_0 = 0$ and $x_1 = 1$,

$$L_0(x) = 1 - x\,, \quad L_1(x) = x\,,$$

and then,

$$\begin{aligned} H_1(x) &= [L_1(x)]^2(1 - 2L'_1(x_1)(x - x_1)) = x^2(3 - 2x)\,, \\ K_0(x) &= [L_0(x)]^2(x - x_0) = (1 - x)^2 x\,. \end{aligned}$$

These yield the required Hermite interpolation polynomial,

$$p_3(x) = -x^3 + x^2 + x\,.$$

◇

Definition 6.4 *Suppose that f is a real-valued function, defined on the closed interval $[a,b]$ of $\mathbb{R}$, and that f is continuous and differentiable on this interval. Suppose, further, that $n \geq 0$ and that x_i, $i = 0,\ldots,n$, are distinct points in $[a,b]$. Then, the polynomial p_{2n+1} defined by*

$$\boxed{p_{2n+1}(x) = \sum_{k=0}^{n} [H_k(x) f(x_k) + K_k(x) f'(x_k)] \qquad (6.16)}$$

is the **Hermite interpolation polynomial of degree** $2n+1$ **with interpolation points** x_i, $i = 0,\ldots,n$, **for** f. *It satisfies the conditions*

$$p_{2n+1}(x_i) = f(x_i)\,, \quad p'_{2n+1}(x_i) = f'(x_i)\,, \quad i = 0,\ldots,n\,.$$

Pictorially, the graph of p_{2n+1} touches the graph of the function f at the points x_i, $i = 0,\ldots,n$.

To conclude this section we state a result, analogous to Theorem 6.2, concerning the error in Hermite interpolation.

Theorem 6.4 *Suppose that $n \geq 0$ and let f be a real-valued function, defined, continuous and $2n+2$ times differentiable on the interval $[a,b]$, such that $f^{(2n+2)}$ is continuous on $[a,b]$. Further, let p_{2n+1} denote the Hermite interpolation polynomial of f defined by (6.16). Then, for each $x \in [a,b]$ there exists $\xi = \xi(x)$ in (a,b) such that*

$$f(x) - p_{2n+1}(x) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}[\pi_{n+1}(x)]^2\,, \qquad (6.17)$$

where π_{n+1} is as defined in (6.9). Moreover,

$$|f(x) - p_{2n+1}(x)| \leq \frac{M_{2n+2}}{(2n+2)!}[\pi_{n+1}(x)]^2\,, \qquad (6.18)$$

where $M_{2n+2} = \max_{\zeta\in[a,b]} |f^{(2n+2)}(\zeta)|$.

Proof The inequality (6.18) is a straightforward consequence of (6.17). In order to prove (6.17), we observe that it is trivially true if $x = x_i$

for some i, $i = 0, \ldots, n$; thus, it suffices to consider $x \in [a, b]$ such that $x \neq x_i$, $i = 0, \ldots, n$. For such x, let us define the function $t \mapsto \psi(t)$ by

$$\psi(t) = f(t) - p_{2n+1}(t) - \frac{f(x) - p_{2n+1}(x)}{[\pi_{n+1}(x)]^2}[\pi_{n+1}(t)]^2 .$$

Then, $\psi(x_i) = 0$ for $i = 0, \ldots, n$, and also $\psi(x) = 0$. Hence, by Rolle's Theorem, $\psi'(t)$ vanishes at $n+1$ points which lie strictly between each pair of consecutive points from the set $\{x_0, \ldots, x_n, x\}$. Also $\psi'(x_i) = 0$, $i = 0, \ldots, n$; hence ψ' vanishes at a total of $2n+2$ distinct points in $[a, b]$. Applying Rolle's Theorem repeatedly, we find eventually that $\psi^{(2n+2)}$ vanishes at some point ξ in (a, b), the location of ξ being dependent on the position of x. This gives the required result on computing $\psi^{(2n+2)}(t)$ from the definition of ψ above and noting that $\psi^{(2n+2)}(\xi) = 0$ and $p_{2n+1}^{(2n+2)}(t) \equiv 0$. $\square$

6.5 Differentiation

From the Lagrange interpolation polynomial p_n, defined by (6.7), which is an approximation to f, it is easy to obtain the polynomial p_n', which is an approximation to the derivative f'. The polynomial p_n' is given by

$$p_n'(x) = \sum_{k=0}^{n} L_k'(x)\, f(x_k)\,, \qquad n \geq 1\,. \tag{6.19}$$

The degree of the polynomial p_n' is clearly at most $n-1$; p_n' is a linear combination of the derivatives of the polynomials $L_k \in \mathcal{P}_n$, the coefficients being the values of f at the interpolation points x_k, $k = 0, 1, \ldots, n$.

In order to find an expression for the difference between $f'(x)$ and the approximation $p_n'(x)$, we might simply differentiate (6.8) to give

$$f'(x) - p_n'(x) = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,\pi_{n+1}(x)\right) .$$

However, the result is not helpful: on application of the chain rule, the right-hand side involves the derivative $\mathrm{d}\xi/\mathrm{d}x$; the value of ξ depends on x, but not in any simple manner. In fact, it is not *a priori* clear that the function $x \mapsto \xi(x)$ is continuous, let alone differentiable. An alternative approach is given by the following theorem.

Theorem 6.5 *Let $n \geq 1$, and suppose that f is a real-valued function defined and continuous on the closed real interval $[a, b]$, such that the derivative of order $n+1$ of f is continuous on $[a, b]$. Suppose further that*

x_i, $i = 0, 1, \ldots, n$, are distinct points in $[a, b]$, and that $p_n \in \mathcal{P}_n$ is the Lagrange interpolation polynomial for f defined by these points. Then, there exist distinct points η_i, $i = 1, \ldots, n$, in (a, b), and corresponding to each x in $[a, b]$ there exists a point $\xi = \xi(x)$ in (a, b), such that

$$f'(x) - p_n'(x) = \frac{f^{(n+1)}(\xi)}{n!} \pi_n^*(x)\,, \tag{6.20}$$

where

$$\pi_n^*(x) = (x - \eta_1) \ldots (x - \eta_n)\,.$$

Proof Since $f(x_i) - p_n(x_i) = 0$, $i = 0, 1, \ldots, n$, there exists a point η_i in (x_{i-1}, x_i) at which $f'(\eta_i) - p_n'(\eta_i) = 0$, for each $i = 1, \ldots, n$. This defines the points η_i, $i = 1, \ldots, n$. Now the proof closely follows that of Theorem 6.2.

When $x = \eta_i$ for some $i \in \{1, \ldots, n\}$, both sides of (6.20) are zero. Suppose then that x is distinct from all the η_i, $i = 1, \ldots, n$, and define the function $t \mapsto \chi(t)$ by

$$\chi(t) = f'(t) - p_n'(t) - \frac{f'(x) - p_n'(x)}{\pi_n^*(x)} \pi_n^*(t)\,.$$

This function vanishes at every point η_i, $i = 1, \ldots, n$, and also at the point $t = x$. By successively applying Rolle's Theorem we deduce that $\chi^{(n)}$ vanishes at some point ξ. The result then follows as in the proof of Theorem 6.2. □

Corollary 6.1 *Under the conditions of Theorem 6.5,*

$$|f'(x) - p_n'(x)| \le \frac{M_{n+1}}{n!} |\pi_n^*(x)| \le \frac{(b-a)^n\, M_{n+1}}{n!}$$

for all x in $[a, b]$, where $M_{n+1} = \max_{x \in [a,b]} |f^{(n+1)}(x)|$.

In particular, we deduce that if f and all its derivatives are defined and continuous on the closed interval $[a, b]$, and

$$\lim_{n \to \infty} \frac{(b-a)^n\, M_{n+1}}{n!} = 0\,,$$

then $\lim_{n \to \infty} \max_{x \in [a,b]} |f'(x) - p_n'(x)| = 0$, showing the convergence of the sequence of interpolation polynomials (p_n') to f', uniformly on $[a, b]$.

The discussion in the last few paragraphs may give the impression that numerical differentiation is a straightforward procedure. In practice, however, things are much more complicated since the function values $f(x_i)$, $i = 0, 1, \ldots, n$, will be polluted by rounding errors.

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Example 6.3 *Consider, for example, a real-valued function f that is defined, continuous and differentiable on the closed interval $[-h, h]$ of the real line, where $h > 0$. Suppose that f has been sampled at the points $x_0 = -h$ and $x_1 = h$, and that $f(\pm h)$ are known, but only up to rounding errors $\varepsilon_\pm$, respectively. Consider the Lagrange interpolation polynomial $p_1 \in \mathcal{P}_1$ for f that passes through the points $(-h, f(-h))$ and $(h, f(h))$; clearly,*

$$p_1(x) = \frac{f(h) - f(-h)}{2h}(x + h) + f(-h)\,.$$

Differentiating this with respect to x yields

$$p_1'(x) \equiv \frac{f(h) - f(-h)}{2h}\,.$$

Now, p_1' is a polynomial of degree 0, representing an approximation to $f'(x)$ at any $x \in [-h, h]$, and in particular to $f'(0)$. Unfortunately, in the presence of rounding errors only $f(-h)+\varepsilon_-$ and $f(h)+\varepsilon_+$ are available, with $\varepsilon_\pm$ unknown; thus, we can only calculate

$$\frac{(f(h) + \varepsilon_+) - (f(-h) + \varepsilon_-)}{2h}\,. \tag{6.21}$$

Rewriting this in the form

$$\frac{f(h) - f(-h)}{2h} + \frac{\varepsilon_+ - \varepsilon_-}{2h}\,,$$

we see that even though the first fraction converges to $f'(0)$ as the spacing $2h$ between the interpolation points $-h$ and h tends to 0, for $\varepsilon_+ - \varepsilon_-$ nonzero and fixed the second fraction will tend to infinity as $h \to 0$. Thus, if h is too small in comparison with $|\varepsilon_+ - \varepsilon_-|$, our approximation to $f'(0)$ will be polluted by a large error of size $|\varepsilon_+ - \varepsilon_-|/(2h)$, whereas if h is very large in comparison with $|\varepsilon_+ - \varepsilon_-|$, then $|\varepsilon_+ - \varepsilon_-|/(2h)$ will be small, but $(f(h) - f(-h))/(2h)$ may be a poor approximation to the value $f'(0)$. These observations indicate the existence of an 'optimal' h, depending on the size of the rounding error, for which the error between $f'(0)$ and the approximation (6.21) is smallest. (See Exercise 12 for further details.) ◇

Convergence, as $h \to 0$, of the expression $p_1'(x) \equiv (f(h) - f(-h))/(2h)$ to $f'(0)$ in the last example should not be confused with convergence, as $n \to \infty$, of the sequence of polynomials (p_n') to the function f' discussed just prior to the example. In the former case, the polynomial degree is fixed and the spacing between the two interpolation points, $x_0 = -h$

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and $x_1 = h$, tends to 0; in the latter case, the degree of the polynomial p_n' tends to infinity and consequently the spacing between the increasing number of consecutive interpolation points shrinks. Nevertheless, Example 6.3 illustrates the issue that caution should be exercised in the course of numerical differentiation when rounding errors are present.

6.6 Notes

The interpolation polynomial (6.6) was discovered by Edward Waring (1736–1798) in 1776, rediscovered by Euler in 1783 and published by Joseph-Louis Lagrange (1736–1813) in his *Leçons élémentaires sur les mathématiques*, Paris, 1795.

Lagrange's interpolation theorem is a purely algebraic result, and it also holds in number fields different from the field of real numbers considered in this chapter. In particular, it holds if the numbers x_i and y_i, $i = 0, 1, \ldots, n$, are complex, and the polynomial p_n has complex coefficients. Theorem 6.2 is due to Augustin-Louis Cauchy (1789–1857). The interpolation polynomial (6.15) was discovered by Charles Hermite (1822–1901).

Before modern computers came into general use about 1960, the evaluation of a standard mathematical function for a given value of x required the use of published tables of the function, in book form. If x was not one of the tabulated values, the required result was obtained by interpolation, using tabulated values close to x. The tabulated values were given at equally spaced points, so that usually $x_j = jh$, where h is a fixed increment. In this case the Lagrange formula can be simplified; as this sort of interpolation had to be done frequently, various devices were used to make the calculations easy and quick. Older books, such as F.B. Hildebrand's *Introduction to Numerical Analysis*, published in 1956, contain extensive discussions of such special methods of interpolation, some of which date back to the time of Newton, but are now mainly of historical interest. A notable early contribution to the development of mathematical tables is the work of Henry Briggs (1560–1630), Savilian Professor of Geometry and fellow of Merton College in Oxford, entitled *Arithmetica logarithmica*, published in 1624. It contained extensive calculations of the logarithms of thirty thousand numbers to 14 decimal digits; these were the numbers from 1 to 20000 and from 90000 to 100000. It also contained tables of the sin function to 15 decimal digits, and of the tan and sec functions to 10 decimal digits.

Exercises

6.1 Construct the Lagrange interpolation polynomial p_1 of degree 1, for a continuous function f defined on the interval $[-1,1]$, using the interpolation points $x_0 = -1$, $x_1 = 1$. Show further that if the second derivative of f exists and is continuous on $[0,1]$, then

$$|f(x) - p_1(x)| \le \frac{M_2}{2}(1 - x^2) \le \frac{M_2}{2}\,, \quad x \in [-1,1]\,,$$

where $M_2 = \max_{x\in[-1,1]} |f''(x)|$. Give an example of a function f, and a point x, for which equality is achieved.

6.2 (i) Write down the Lagrange interpolation polynomial of degree 1 for the function $f\colon x \mapsto x^3$, using the points $x_0 = 0$, $x_1 = a$. Verify Theorem 6.2 by direct calculation, showing that in this case ξ is unique and has the value $\xi = \frac{1}{3}(x + a)$.

(ii) Repeat the calculation for the function $f\colon x \mapsto (2x - a)^4$; show that in this case there are two possible values for ξ, and give their values.

6.3 Given the distinct points x_i, $i = 0, 1, \ldots, n+1$, and the points y_i, $i = 0, 1, \ldots, n+1$, let q be the Lagrange polynomial of degree n for the set of points $\{(x_i, y_i)\colon i = 0, 1, \ldots, n\}$ and let r be the Lagrange polynomial of degree n for the points $\{(x_i, y_i)\colon i = 1, 2, \ldots, n+1\}$. Define

$$p(x) = \frac{(x - x_0)r(x) - (x - x_{n+1})q(x)}{x_{n+1} - x_0}\,.$$

Show that p is the Lagrange polynomial of degree $n+1$ for the points $\{(x_i, y_i)\colon i = 0, 1, \ldots, n+1\}$.

6.4 Let $n \ge 1$. The points x_j are equally spaced in $[-1,1]$, so that

$$x_j = \frac{2j - n}{n}\,, \quad j = 0, \ldots, n\,.$$

With the usual notation

$$\pi_{n+1}(x) = (x - x_0)\ldots(x - x_n),$$

show that

$$\pi_{n+1}(1 - 1/n) = -\frac{(2n)!}{2^n n^{n+1} n!}\,.$$

Using Stirling's formula

$$N! \sim \sqrt{2\pi} N^{N+1/2} \mathrm{e}^{-N}\,, \qquad N \to \infty\,,$$

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verify that

$$\pi_{n+1}(1 - 1/n) \sim -\frac{2^{n+1/2}\mathrm{e}^{-n}}{n}$$

for large values of n.

6.5 Let $n \geq 1$. Suppose that x_i, $i = 0, 1, \ldots, n$, are distinct real numbers, and y_i, u_i, $i = 0, 1, \ldots, n$, are real numbers. Suppose, further, that there exists $p_{2n+1} \in \mathcal{P}_{2n+1}$ such that $p_{2n+1}(x_i) = y_i$ for all $i = 0, 1, \ldots, n$, and $p''_{2n+1}(x_i) = u_i$, $i = 0, 1, \ldots, n$. Attempt to prove that p_{2n+1} is the unique polynomial with these properties, by adapting the uniqueness proofs in Sections 6.2 and 6.4, using Rolle's Theorem; explain where the proof fails. Show that there is no polynomial $p_5 \in \mathcal{P}_5$ such that $p_5(-1) = 1$, $p_5(0) = 0$, $p_5(1) = 1$, $p''_5(-1) = 0$, $p''_5(0) = 0$, $p''_5(1) = 0$, but that if the first condition is replaced by $p_5(-1) = -1$, then there is an infinite number of such polynomials. Give an explicit expression for the general form of these polynomials.

6.6 Suppose that $n \geq 1$. The function f and its derivatives of order up to and including $2n + 1$ are continuous on $[a, b]$. The points x_i, $i = 0, 1, \ldots, n$, are distinct and lie in $[a, b]$. Construct polynomials $l_0(x)$, $h_i(x)$, $k_i(x)$, $i = 1, \ldots, n$, of degree $2n$ such that the polynomial

$$p_{2n}(x) = l_0(x)f(x_0) + \sum_{i=1}^{n}[h_i(x)f(x_i) + k_i(x)f'(x_i)]$$

satisfies the conditions

$$p_{2n}(x_i) = f(x_i)\,, \quad i = 0, 1, \ldots, n\,,$$

and

$$p'_{2n}(x_i) = f'(x_i)\,, \quad i = 1, \ldots, n\,.$$

Show also that for each value of x in $[a, b]$ there is a number η, depending on x, such that

$$f(x) - p_{2n}(x) = \frac{(x - x_0)\prod_{i=1}^{n}(x - x_i)^2}{(2n + 1)!} f^{(2n+1)}(\eta)\,.$$

6.7 Suppose that $n \geq 2$. The function f and its derivatives of order up to and including $2n$ are continuous on $[a, b]$. The points x_i, $i = 0, 1, \ldots, n$, are distinct and lie in $[a, b]$. Explain how to

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construct polynomials $l_0(x)$, $l_n(x)$, $h_i(x)$, $k_i(x)$, $i = 1, \ldots, n-1$, of degree $2n - 1$ such that the polynomial

$$p_{2n-1}(x) = l_0(x) f(x_0) + l_n(x) f(x_n) + \sum_{i=1}^{n-1} [h_i(x) f(x_i) + k_i(x) f'(x_i)]$$

satisfies the conditions $p_{2n-1}(x_i) = f(x_i)$, $i = 0, 1, \ldots, n$, and $p'_{2n-1}(x_i) = f'(x_i)$, $i = 1, \ldots, n-1$. It is not necessary to give explicit expressions for these polynomials.

Show also that for each value of x in $[a, b]$ there is a number η, depending on x, such that

$$f(x) - p_{2n-1}(x) = \frac{(x - x_0)(x - x_n) \prod_{i=1}^{n-1} (x - x_i)^2}{(2n)!} f^{(2n)}(\eta)\,.$$

6.8 By considering the symmetry of the graph of the polynomial

$$q(x) = x(x^2 - 1)(x^2 - 4)(x - 3)\,,$$

show that the maximum of $|q(x)|$ over the interval $[0, 1]$ is attained at the point $x = \frac{1}{2}$.

The values of the function $f\colon x \mapsto \sin x$ are given at the points $x_i = i\pi/8$, for all integer values of i. For a general value of x, an approximation $u(x)$ to $f(x)$ is calculated by first defining k to be the integer part of $8x/\pi$, so that $x_k \le x \le x_{k+1}$, and then evaluating the Lagrange polynomial of degree 5 using the six interpolation points $(x_j, f(x_j))$, $j = k-2, \ldots, k+3$. Show that, for all values of x,

$$|\sin x - u(x)| \le \frac{225\,\pi^6}{16^6 \times 6!} < 0.00002\,.$$

6.9 Let $n \ge 1$. The interpolation points x_j, $j = 0, 1, \ldots, 2n-1$, are distinct, and $x_{n+j} = x_j + \varepsilon$ for each $j = 0, \ldots, n-1$. The Lagrange polynomial of degree $2n - 1$ for the function f using these points is denoted by p_{2n-1}. Show that the terms involving $f(x_j)$ and $f(x_{n+j})$ in p_{2n-1} may be written

$$\frac{\varphi_j(x)\,\varphi_j(x - \varepsilon)}{\varepsilon\,\varphi_j(x_j)} \left\{ \frac{x - x_j}{\varphi_j(x_j + \varepsilon)} f(x_j + \varepsilon) - \frac{x - x_j - \varepsilon}{\varphi_j(x_j - \varepsilon)} f(x_j) \right\},$$

where

$$\varphi_j(x) = \prod_{\substack{i=0 \\ i \ne j}}^{n-1} (x - x_i)\,.$$

Find the limit of this expression as $\varepsilon \to 0$, and deduce that $p_{2n-1} - q_{2n-1} \to 0$ as $\varepsilon \to 0$, where q_{2n-1} is the Hermite interpolation polynomial for f, using the points x_i, $i = 0, \dots, n-1$.

6.10 Construct the Hermite interpolation polynomial of degree 3 for the function $f\colon x \mapsto x^5$, using the points $x_0 = 0$, $x_1 = a$, and show that it has the form $p_3(x) = 3a^2x^3 - 2a^3x^2$. Verify Theorem 6.4 by direct calculation, showing that in this case ξ is unique and has the value $\xi = \frac{1}{5}(x + 2a)$.

6.11 The complex function $z \mapsto f(z)$ of the complex variable z is holomorphic in the region D of the complex plane; the boundary of D is the simple closed contour C. The interpolation points x_j, $j = 0, 1, \dots, n$, with $n \geq 1$, and the point x all lie in D. Determine the residues of the function g defined by

$$g(z) = \frac{f(z)}{z - x} \prod_{j=0}^{n} \frac{x - x_j}{z - x_j}$$

at its poles in D, and deduce that

$$f(x) - p_n(x) = \frac{1}{2\pi\imath} \int_C \frac{f(z)}{z - x} \prod_{j=0}^{n} \frac{x - x_j}{z - x_j} \mathrm{d}z\,,$$

where p_n is the Lagrange interpolation polynomial for the function f using the interpolation points x_j, $j = 0, 1, \dots, n$.

Now, suppose that the real number x and the interpolation points x_j, $j = 0, 1, \dots, n$, all lie in the real interval $[a, b]$, and that D consists of all the points z such that $|z - t| < K$ for all $t \in [a, b]$, where K is a constant with $K > |b - a|$. Show that the length of the contour C is $2(b - a) + 2\pi K$, and that

$$|f(x) - p_n(x)| < \frac{(b - a + \pi K)M}{\pi} \left(\frac{b - a}{K}\right)^{n+1},$$

where M is such that $|f(z)| \leq M$ on C. Deduce that the sequence (p_n) converges to f, uniformly on $[a, b]$.

Show that these conditions are not satisfied by the function $f\colon x \mapsto 1/(1 + x^2)$ for x in the interval $[-5, 5]$. For what values of a are the conditions satisfied by f for x in the interval $[-a, a]$?

6.12 With the same notation as in Example 6.3, let

$$E(h) = \frac{(f(h) + \varepsilon_+) - (f(-h) + \varepsilon_-)}{2h} - f'(0)\,.$$

Suppose that $f'''(x)$ exists and is continuous at all $x \in [-h, h]$.

By expanding $f(h)$ and $f(-h)$ into Taylor series about the point 0, show that there exists $\xi \in (-h, h)$ such that

$$E(h) = \frac{1}{6}h^2 f'''(\xi) + \frac{\varepsilon_+ - \varepsilon_-}{2h}\,.$$

Hence deduce that

$$|E(h)| \leq \frac{1}{6}h^2 M_3 + \frac{\varepsilon}{h}$$

where $M_3 = \max_{x \in [-h,h]} |f'''(x)|$ and $\varepsilon = \max(|\varepsilon_+|, |\varepsilon_-|)$. Show further that the right-hand side of the last inequality achieves its minimum value when

$$h = \left(\frac{3\varepsilon}{M_3}\right)^{1/3}\,.$$

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