

4. INTERPOLATION

Given that

$$y = f(x), \quad x_0 \leq x \leq x_n$$

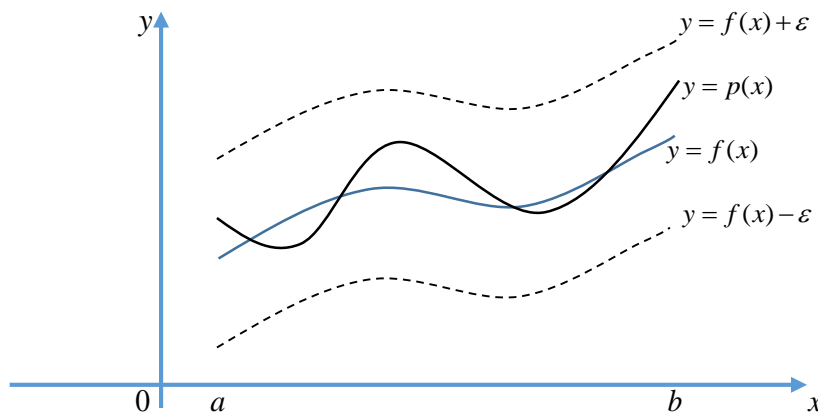
and assuming that $f(x)$ is single-valued, continuous and explicitly known, then the value of $f(x)$ corresponding to x_0, x_1, \dots, x_n can easily be computed and tabulated. Suppose we want to reverse this process, that is, given the set of tabular values $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ satisfying the relation $y = f(x)$, where the explicit nature of $f(x)$ is not known, we want to find a simpler function, say $\phi(x)$, such that $f(x)$ and $\phi(x)$ agree at the set of tabulated points. Such a process is called interpolation. If $\phi(x)$ is a polynomial, then the process is called polynomial interpolation. One reason for approximating unknown function by means of a polynomial is outlined in the following theorem:

Theorem 4.1.1 (Weierstrass Approximation Theorem)

Suppose that f is defined and continuous on $[a, b]$. For each $\varepsilon > 0$, there exists a polynomial $p(x)$, with the property that

$$|f(x) - p(x)| < \varepsilon, \quad \text{for all } x \in [a, b]. \quad \square$$

Theorem 4.1.1 shows that given any function, defined and continuous on a closed and bounded interval, there exists a polynomial that is as “close” to the given function as desired.



The fact that derivatives and indefinite integrals for polynomials can easily be determined is another reason for using polynomials to approximate unknown function.

Taylor polynomial may not give a correct approximation because it is concentrated at a point x_0 . Thus, moving away from x_0 gives inaccurate approximations.

Exercise: Check that using the Taylor polynomial for $f(x) = \frac{1}{x}$ expanded about $x = 1$ to

approximate $f(3) = \frac{1}{3}$ gives inaccurate value.

4. 1. LAGRANGE INTERPOLATING POLYNOMIAL

Suppose we have two distinct points (x_0, y_0) and (x_1, y_1) , and would like to approximate f for which $f(x_0) = y_0$ and $f(x_1) = y_1$. Define the functions

$$L_0(x) = \frac{x - x_1}{x_0 - x_1} \quad \text{and} \quad L_1(x) = \frac{x - x_0}{x_1 - x_0}.$$

The linear Lagrange interpolating polynomial through (x_0, y_0) and (x_1, y_1) is

$$p(x) = L_0(x)f(x_0) + L_1(x)f(x_1) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

Example 4.1.1

Determine the linear interpolating polynomial that passes through the points $(2, 4)$ and $(5, 1)$.

Solution:

$$L_0(x) = \frac{x - x_1}{x_0 - x_1} = \frac{x - 5}{2 - 5} = -\frac{1}{3}(x - 5)$$

$$L_1(x) = \frac{x - x_0}{x_1 - x_0} = \frac{x - 2}{5 - 2} = \frac{1}{3}(x - 2)$$

$$\begin{aligned} \therefore p(x) &= L_0(x)f(x_0) + L_1(x)f(x_1) = \left(-\frac{1}{3}(x - 5)\right)(4) + \left(\frac{1}{3}(x - 2)\right)(1) \\ &= -x + 6 \end{aligned}$$

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Questions: 1. What happens when you “swap” points?

2. What do the values $p(x_0)$ and $p(x_1)$ show?

NOTE: Two points give a linear function (polynomial of degree 1). It follows that $n + 1$ points give a polynomial of degree at most n .

Suppose that we have $n+1$ points $(x_0, f(x_0)), (x_1, f(x_1)), \dots, (x_n, f(x_n))$. In this case, we first construct $L_{n,k}(x)$, for $k = 0, 1, 2, \dots, n$ with the property that

$$L_{n,k}(x_i) = \begin{cases} 1, & \text{if } i = k \\ 0, & \text{if } i \neq k \end{cases}.$$

For example, from Example 4.1.1,

$$L_{1,0}(x_0) = L_{1,0}(2) = -\frac{1}{3}(2-5) = 1$$

$$L_{1,0}(x_1) = L_{1,0}(5) = -\frac{1}{3}(5-5) = 0$$

$$L_{1,1}(x_0) = L_{1,1}(2) = \frac{1}{3}(2-2) = 0$$

$$L_{1,1}(x_1) = L_{1,1}(5) = \frac{1}{3}(5-2) = 1.$$

To satisfy $L_{n,k}(x_i) = 0, i \neq k$, requires that the numerator of $L_{n,k}(x)$ contain the term

$$(x-x_0)(x-x_1)\dots(x-x_{k-1})(x-x_{k+1})\dots(x-x_n),$$

and $L_{n,k}(x_i) = 1, i = k$, requires that the denominator be evaluated at $x = x_k$. Thus,

$$L_{n,k}(x) = \frac{(x-x_0)(x-x_1)\dots(x-x_{k-1})(x-x_{k+1})\dots(x-x_n)}{(x_k-x_0)(x_k-x_1)\dots(x_k-x_n)},$$

for example, when $n = 2$,

$$L_{2,0}(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}$$

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

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

The n^{th} Lagrange interpolating polynomial is defined in the following theorem:

Theorem 4.1.2

If x_0, x_1, \dots, x_n are $n+1$ distinct numbers and f is a function whose values are given at these numbers, then a unique polynomial $p(x)$ at most n exists with

$$f(x_k) = p(x_k), \text{ for each } k = 0, 1, 2, \dots, n.$$

This polynomial is given by

$$\begin{aligned} p(x) &= f(x_0)L_{n,0}(x) + f(x_1)L_{n,1}(x) + \dots + f(x_{n-1})L_{n,n-1}(x) + f(x_n)L_{n,n}(x) \\ &= \sum_{k=0}^n f(x_k)L_{n,k}(x), \end{aligned}$$

where for each $k = 0, 1, 2, \dots, n$,

$$\begin{aligned} L_{n,k}(x) &= \frac{(x-x_0)(x-x_1)\dots(x-x_{k-1})(x-x_{k+1})\dots(x-x_n)}{(x_k-x_0)(x_k-x_1)\dots(x_k-x_n)} \\ &= \prod_{\substack{i=0 \\ i \neq k}}^n \frac{(x-x_i)}{(x_k-x_i)}. \end{aligned}$$

The numbers x_0, x_1, \dots, x_n are called nodes. □

Example 4.1.2

Use the nodes $x_0 = 2$, $x_1 = 2.75$ and $x_2 = 4$ to find the second Lagrange interpolating polynomial for $f(x) = \frac{1}{x}$ and use it to approximate $f(3) = \frac{1}{3}$.

Solution:

$$\begin{aligned} L_{2,0}(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-2.75)(x-4)}{(2-2.75)(2-4)} = \frac{2}{3}(x-2.75)(x-4) \\ L_{2,1}(x) &= \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-2)(x-4)}{(2.75-2)(2.75-4)} = -\frac{16}{15}(x-2)(x-4) \\ L_{2,2}(x) &= \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-2)(x-2.75)}{(4-2)(4-2.75)} = \frac{2}{5}(x-2)(x-2.75) \\ \therefore p(x) &= f(x_0)L_{2,0}(x) + f(x_1)L_{2,1}(x) + f(x_2)L_{2,2}(x) \\ &= \frac{1}{2} \cdot \frac{2}{3}(x-2.75)(x-4) + \frac{4}{11} \cdot -\frac{16}{15}(x-2)(x-4) + \frac{1}{4} \cdot \frac{2}{5}(x-2)(x-2.75) \\ &= \frac{1}{3}(x-2.75)(x-4) - \frac{64}{165}(x-2)(x-4) + \frac{1}{10}(x-2)(x-2.75) \\ &= \frac{1}{22}x^2 - \frac{35}{88}x + \frac{49}{44}. \end{aligned}$$

At $x = 3$,

$$f(3) = \frac{1}{22}(3^2) - \frac{35}{88}(3) + \frac{49}{44} = \frac{29}{88} \approx 0.32955.$$

△

Theorem 4.1.3

Suppose the nodes in the interval $[a, b]$ are distinct and $f \in C^{n+1}[a, b]$. Then, for each x in $[a, b]$, a number $\xi(x)$ (generally unknown) between the nodes, and hence in (a, b) exists with

$$f(x) = p(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} (x-x_0)(x-x_1)\dots(x-x_n),$$

where $p(x)$ is the n^{th} Lagrange interpolating polynomial. □

NOTE: The error formula given in Theorem 4.1.3 is similar to that given by the Taylor Theorem, only that this error uses information at the distinct numbers x_0, x_1, \dots, x_n .

Example 4.1.3

Find the error formula for the second Lagrange interpolating polynomial found in Example 4.1.2 and find the maximum error when this polynomial is used to approximate $f(x)$ for x in $[2, 4]$.

Solution:

$$f(x) = \frac{1}{x} \Rightarrow f'(x) = -\frac{1}{x^2}, f''(x) = \frac{2}{x^3}, f'''(x) = -\frac{6}{x^4}.$$

Thus,

$$f(x) = p(x) + \frac{f^{(3)}(\xi(x))}{(2+1)!} (x-x_0)(x-x_1)(x-x_2),$$

where

$$\begin{aligned} \frac{f^{(3)}(\xi(x))}{3!} (x-x_0)(x-x_1)(x-x_2) &= -\frac{6}{6(\xi(x))^4} (x-2)(x-2.75)(x-4) \\ &= -(\xi(x))^{-4} (x-2)(x-2.75)(x-4), \text{ for } \xi(x) \text{ in } (2,4). \end{aligned}$$

The maximum value of $(\xi(x))^{-4}$ on $(2,4)$ is $2^{-4} = \frac{1}{16}$. We now determine the maximum value

of the absolute value of the polynomial $g(x) = (x-2)(x-2.75)(x-4) = x^3 - \frac{35}{4}x^2 + \frac{49}{2}x - 22$

$$g'(x) = 0 \Rightarrow 3x^2 - \frac{35}{2}x + \frac{49}{2} = 0 \Rightarrow x = \frac{7}{3} \text{ or } x = \frac{7}{2}$$

$$\therefore g\left(\frac{7}{3}\right) = \frac{25}{108} \text{ or } g\left(\frac{7}{2}\right) = -\frac{9}{16}.$$

Hence, the maximum error is $\left| \frac{f^{(3)}(\xi(x))}{3!} g(x) \right| \leq \left| \frac{1}{16} \right| \left| -\frac{9}{16} \right| = \frac{9}{256} \approx 0.0352$.

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4.2. DIVIDED DIFFERENCES

Suppose that $p_n(x)$ is the n^{th} Lagrange interpolating polynomial that agrees with the function f at distinct numbers x_0, x_1, \dots, x_n . The divided differences of f with respect to x_0, x_1, \dots, x_n are used to express $p_n(x)$ in the form

$$p_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \dots + a_n(x - x_0)(x - x_1)\dots(x - x_{n-1})$$

for some constants a_0, a_1, \dots, a_n . Note that

$$\begin{aligned} p_n(x_0) &= a_0 = f(x_0) \\ p_n(x_1) &= a_0 + a_1(x_1 - x_0) = f(x_1) \Rightarrow a_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}. \end{aligned}$$

The zeroth divided difference of f with respect to x_i , denoted $f[x_i]$, is $f[x_i] = f(x_i)$.

The first divided difference of f with respect to x_i and x_{i+1} , denoted $f[x_i, x_{i+1}]$, is

$$f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}.$$

The second divided difference is

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}.$$

Similarly, the k^{th} divided difference relative to $x_i, x_{i+1}, x_{i+2}, \dots, x_{i+k}$, is

$$f[x_i, x_{i+1}, x_{i+2}, \dots, x_{i+k}] = \frac{f[x_{i+1}, x_{i+2}, \dots, x_{i+k}] - f[x_i, x_{i+1}, x_{i+2}, \dots, x_{i+k-1}]}{x_{i+k} - x_i}.$$

This process ends with a single n^{th} divided difference

$$f[x_0, x_1, \dots, x_n] = \frac{f[x_1, x_2, \dots, x_n] - f[x_0, x_1, \dots, x_{n-1}]}{x_n - x_0}.$$

Thus, $p_n(x)$ can be written as

$$\begin{aligned} p_n(x) &= f[x_0] + f[x_0, x_1](x - x_0) + \dots + f[x_0, x_1, \dots, x_n](x - x_0)(x - x_1)\dots(x - x_{n-1}) \\ &= f[x_0] + \sum_{k=1}^n f[x_0, x_1, \dots, x_k](x - x_0)(x - x_1)\dots(x - x_{k-1}) \end{aligned} \quad (4.1)$$

Equation (4.1) is known as Newton's Divided-Difference formula. The table below outlines how divided differences from tabulated data can be determined:

x	$f(x)$	1^{st}	2^{nd}	3^{rd}
x_0	$f[x_0]$			
x_1	$f[x_1]$	$f[x_0, x_1]$		
x_2	$f[x_2]$	$f[x_1, x_2]$	$f[x_0, x_1, x_2]$	
x_3	$f[x_3]$	$f[x_2, x_3]$	$f[x_1, x_2, x_3]$	$f[x_0, x_1, x_2, x_3]$
\vdots	\vdots			

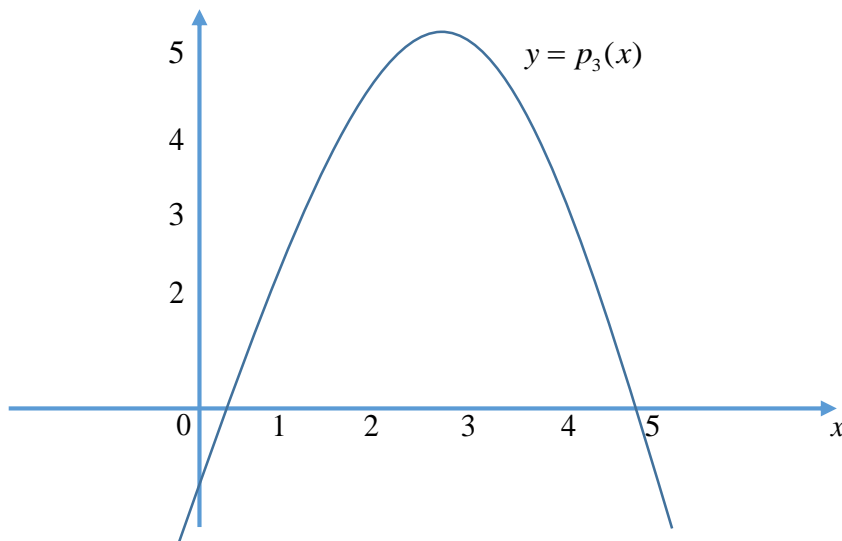
Example 4.2.1

Suppose we have the data $(1, 2), (2, 4), (4, 3), (5, 0)$. Then,

$$x_0 = 1, x_1 = 2, x_2 = 4, x_3 = 5 \text{ and } f[x_0] = 2, f[x_1] = 4, f[x_2] = 3, f[x_3] = 0$$

x	$f(x)$	1^{st}	2^{nd}	3^{rd}
1	$f[x_0] = 2$			
2	$f[x_1] = 4$	$f[x_0, x_1] = \frac{4-2}{2-1} = 2$		
4	$f[x_2] = 3$	$f[x_1, x_2] = \frac{3-4}{4-2} = -\frac{1}{2}$	$f[x_0, x_1, x_2] = \frac{-\frac{1}{2}-2}{4-1} = -\frac{5}{6}$	
5	$f[x_3] = 0$	$f[x_2, x_3] = \frac{0-3}{5-4} = -3$	$f[x_1, x_2, x_3] = \frac{-3-(-\frac{1}{2})}{5-2} = -\frac{5}{6}$	$f[x_0, x_1, x_2, x_3] = \frac{-\frac{5}{6}-(-\frac{5}{6})}{5-1} = 0$

$$\begin{aligned}
p_3(x) &= f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) \\
&= 2 + 2(x - 1) - \frac{5}{6}(x - 1)(x - 2) + 0(x - 1)(x - 2)(x - 4) \\
&= -\frac{5}{3} + \frac{9}{2}x - \frac{5}{6}x^2. \\
\therefore p_3(3) &= -\frac{5}{3} + \frac{9}{2}(3) - \frac{5}{6}(3^2) = 5.1\bar{6}.
\end{aligned}$$



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Example 4.2.2

Write the divided difference table for the given values of x and $f(x)$. Hence, find $p_4(x)$.

x	$f(x)$
1.0	0.7651977
1.3	0.6200860
1.6	0.4554022
1.9	0.2818186
2.2	0.1103623

Solution:

Here $x_0 = 1.0, x_1 = 1.3, x_2 = 1.6, x_3 = 1.9, x_4 = 2.2$

$f[x_0] = 0.7651977, f[x_1] = 0.6200860, f[x_2] = 0.4554022, f[x_3] = 0.2818186, f[x_4] = 0.1103623$

$$\begin{aligned}
f[x_0, x_1] &= \frac{f[x_1] - f[x_0]}{x_1 - x_0} = \frac{0.6200860 - 0.7651977}{1.3 - 1.0} = -0.4837057 \\
f[x_1, x_2] &= \frac{f[x_2] - f[x_1]}{x_2 - x_1} = \frac{0.4554022 - 0.6200860}{1.6 - 1.3} = -0.5489460 \\
f[x_2, x_3] &= \frac{f[x_3] - f[x_2]}{x_3 - x_2} = \frac{0.2818186 - 0.4554022}{1.9 - 1.6} = -0.5786120 \\
f[x_3, x_4] &= \frac{f[x_4] - f[x_3]}{x_4 - x_3} = \frac{0.1103623 - 0.2818186}{2.2 - 1.9} = -0.571521 \\
f[x_0, x_1, x_2] &= \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} = \frac{-0.5489460 - (-0.4837057)}{1.6 - 1.0} = -0.1087338 \\
f[x_1, x_2, x_3] &= \frac{f[x_2, x_3] - f[x_1, x_2]}{x_3 - x_1} = \frac{-0.5786120 - (-0.5489460)}{1.9 - 1.3} = -0.0494433 \\
f[x_2, x_3, x_4] &= \frac{f[x_3, x_4] - f[x_2, x_3]}{x_4 - x_2} = \frac{-0.571521 - (-0.5786120)}{2.2 - 1.6} = 0.0118183 \\
f[x_0, x_1, x_2, x_3] &= \frac{f[x_1, x_2, x_3] - f[x_0, x_1, x_2]}{x_3 - x_0} = \frac{-0.0494433 - (-0.1087338)}{1.9 - 1.0} = 0.0658783 \\
f[x_1, x_2, x_3, x_4] &= \frac{f[x_2, x_3, x_4] - f[x_1, x_2, x_3]}{x_4 - x_1} = \frac{0.0118183 - (-0.0494433)}{2.2 - 1.3} = 0.0680684 \\
f[x_0, x_1, x_2, x_3, x_4] &= \frac{f[x_1, x_2, x_3, x_4] - f[x_0, x_1, x_2, x_3]}{x_4 - x_0} = \frac{0.0680684 - 0.0658783}{2.2 - 1.0} = 0.0018251
\end{aligned}$$

x	$f(x)$	1^{st}	2^{nd}	3^{rd}	4^{th}
1.0	$f[x_0] = 0.7651977$				
		$f[x_0, x_1] = -0.4837057$			
1.3	$f[x_1] = 0.6200860$		$f[x_0, x_1, x_2] = -0.1087338$		
		$f[x_1, x_2] = -0.5489460$		$f[x_0, x_1, x_2, x_3] = 0.0658783$	
1.6	$f[x_2] = 0.4554022$		$f[x_1, x_2, x_3] = -0.0494433$		$f[x_0, x_1, x_2, x_3] = 0.0018251$
		$f[x_2, x_3] = 0.5786120$		$f[x_1, x_2, x_3, x_4] = 0.0680684$	
1.9	$f[x_3] = 0.2818186$		$f[x_2, x_3, x_4] = 0.0118183$		
		$f[x_3, x_4] = -0.5715210$			
2.2	$f[x_4] = 0.1103623$				

$$\begin{aligned}
\therefore p_4(x) &= 0.7651977 - 0.4837057(x - 1.0) - 0.1087338(x - 1.0)(x - 1.3) \\
&\quad + 0.0658783(x - 1.0)(x - 1.3)(x - 1.6) + 0.0018251(x - 1.0)(x - 1.3)(x - 1.6)(x - 1.9)
\end{aligned}$$

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4.2.1. Newton Forward- and Backward-Difference

Let us try to write equation (4.1) in a simplified form when the nodes are arranged consecutively with equal spacing. Let $h = x_{i+1} - x_i$ and $x = x_0 + sh$. Since the nodes are equally spaced, we have that $x_i = x_0 + ih$ which implies that the difference $x - x_i$ is

$$x - x_i = x_0 + sh - (x_0 + ih) = (s - i)h.$$

Thus, equation (4.1) becomes

$$p_n(x) = p_n(x_0 + sh) = f[x_0] + shf[x_0, x_1] + s(s-1)h^2 f[x_0, x_1, x_2] + \dots + s(s-1)\dots(s-n+1)h^n f[x_0, x_1, \dots, x_n].$$

Since $s(s-1)\dots(s-k+1) = k! \binom{s}{k}$, we have that

$$p_n(x) = p_n(x_0 + sh) = f[x_0] + \sum_{k=1}^n \binom{s}{k} k! h^k f[x_0, x_1, \dots, x_k] \quad (4.2)$$

Equation (4.2) is known as Newton Forward-Difference formula.

Newton Backward-Difference formula is obtained when the nodes are reordered from last to first. In this case, (4.1) can be written in the form

$$\begin{aligned} p_n(x) = & f[x_n] + f[x_n, x_{n-1}](x - x_n) + f[x_n, x_{n-1}, x_{n-2}](x - x_n)(x - x_{n-1}) \\ & + \dots + f[x_n, x_{n-1}, \dots, x_0](x - x_n)(x - x_{n-1})\dots(x - x_1). \end{aligned}$$

As observed above, since the nodes are equally spaced, letting $x = x_n + sh$ and $x = x_i + (s + n - i)h$, given

$$\begin{aligned} p_n(x) = p_n(x_n + sh) = & f[x_n] + shf[x_n, x_{n-1}] + s(s+1)h^2 f[x_n, x_{n-1}, x_{n-2}] \\ & + \dots + s(s+1)\dots(s+n-1)h^n f[x_n, x_{n-1}, \dots, x_0]. \end{aligned}$$

If we use

$$\binom{-s}{k} = \frac{-s(-s-1)\dots(-s-k+1)}{k!} = (-1)^k \frac{s(s+1)\dots(s+k-1)}{k!},$$

then the Newton Backward-Difference formula becomes

$$p_n(x) = p_n(x_0 + sh) = f[x_n] + \sum_{k=1}^n \binom{-s}{k} (-1)^k k! h^k f[x_n, x_{n-1}, \dots, x_0] \quad (4.3)$$

NOTE: The Newton Forward- Difference formula is useful for interpolation near the beginning of a set of tabular values and the Newton Backward- Difference formula for interpolation near the end of a set of tabular values.

Example 4.2.3

Use Example 4.2.2 to approximate $f(1.1)$ and $f(2.0)$.

Solution:

Since $x = 1.1$ is near the first value $x_0 = 1.0$, we use The Newton Forward- Difference formula.

Here, $h = 1.3 - 1.0 = 1.6 - 1.3 = 1.9 - 1.6 = 2.2 - 1.9 = 0.3$.

$$x = x_0 + sh \Rightarrow 1.1 = 1.0 + 0.3s \Rightarrow s = \frac{1}{3}.$$

$$\begin{aligned} \therefore f(1.1) &\approx p_4(1.1) = p_4(1.0 + \frac{1}{3}(0.3)) \\ &= 0.7651977 + \frac{1}{3}(0.3)(-0.4837057) + \frac{1}{3}\left(\frac{1}{3} - 1\right)(0.3)^2(-0.1087338) \\ &\quad + \frac{1}{3}\left(\frac{1}{3} - 1\right)\left(\frac{1}{3} - 2\right)(0.3)^3(0.0658783) + \frac{1}{3}\left(\frac{1}{3} - 1\right)\left(\frac{1}{3} - 2\right)\left(\frac{1}{3} - 3\right)(0.3)^4(0.0018251) \\ &= 0.719646. \end{aligned}$$

To approximate $f(2.0)$, we use Newton Backward- Difference formula since $x = 2.0$ is near the last value $x = 2.2$.

$$x = x_n + sh = x_4 + sh \Rightarrow 2.0 = 2.2 + 0.3s \Rightarrow s = -\frac{2}{3}$$

$$\begin{aligned} \therefore f(2.0) &\approx p_4(2.0) = p_4(2.2 - \frac{2}{3}(0.3)) \\ &= 0.1103623 - \frac{2}{3}(0.3)(-0.5715210) - \frac{2}{3}\left(-\frac{2}{3} + 1\right)(0.3)^2(0.0118183) \\ &\quad - \frac{2}{3}\left(-\frac{2}{3} + 1\right)\left(-\frac{2}{3} + 2\right)(0.3)^3(0.0680684) - \frac{2}{3}\left(-\frac{2}{3} + 1\right)\left(-\frac{2}{3} + 2\right)\left(-\frac{2}{3} + 3\right)(0.3)^4(0.0018251) \\ &= 0.2238853. \end{aligned}$$

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4.3. SPLINE INTERPOLATION

One disadvantage of using a single polynomial to approximate an arbitrary function on a closed interval is that high-degree polynomials can oscillate erratically, that is, a minor fluctuation over a small portion of the interval can induce large fluctuations over the entire range. An alternative approach is to divide the approximation interval into a collection of subintervals and construct a (generally) different approximating polynomial on each subinterval. This is called piecewise-polynomial or spline approximation. The splines, which will be denoted by $s_n(x)$, can be classified depending on the order of the polynomials. We will discuss linear, quadratic and cubic splines. Other high-order splines can be derived in a similar way with a greater increase in computational difficulty.

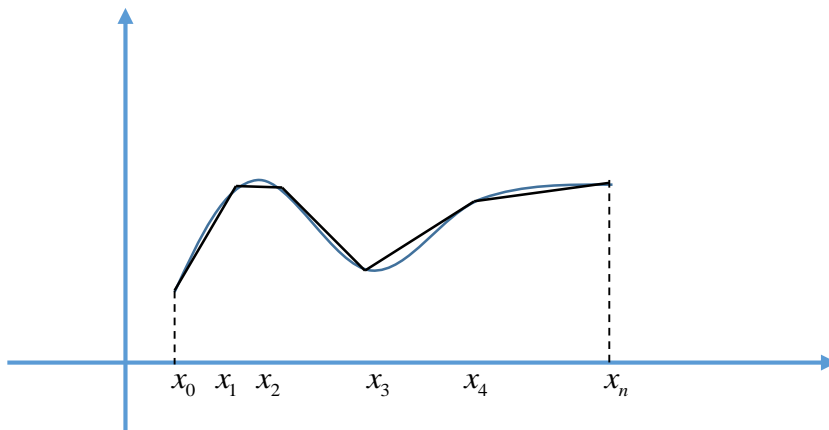
4.3.1. Linear Splines

The simplest spline is a linear spline which consists of joining a set of data points

$$(x_0, f(x_0)), (x_1, f(x_1)), \dots, (x_n, f(x_n)), \quad \text{where } x_0 < x_1 < \dots < x_n,$$

by a series of straight lines such that

$$S(x) = \begin{cases} s_1(x) = f(x_0) \left(\frac{x-x_1}{x_0-x_1} \right) + f(x_1) \left(\frac{x-x_0}{x_1-x_0} \right), & x \in [x_0, x_1] \\ s_2(x) = f(x_1) \left(\frac{x-x_2}{x_1-x_2} \right) + f(x_2) \left(\frac{x-x_1}{x_2-x_1} \right), & x \in [x_1, x_2] \\ \vdots \\ s_n(x) = f(x_{n-1}) \left(\frac{x-x_n}{x_{n-1}-x_n} \right) + f(x_n) \left(\frac{x-x_{n-1}}{x_n-x_{n-1}} \right), & x \in [x_{n-1}, x_n] \end{cases}$$



Example 4.3.1

Construct the linear spline interpolating the data below:

x	-1	0	1
y	0	1	3

Solution:

$$S(x) = \begin{cases} s_1(x), & x \in [-1, 0] \\ s_2(x), & x \in [0, 1] \end{cases}$$

where

$$\begin{aligned} s_1(x) &= f(x_0) \left(\frac{x - x_1}{x_0 - x_1} \right) + f(x_1) \left(\frac{x - x_0}{x_1 - x_0} \right) = f(-1) \left(\frac{x - 0}{-1 - 0} \right) + f(0) \left(\frac{x - (-1)}{0 - (-1)} \right) \\ &= (0) \frac{x}{-1} + (1) \frac{x+1}{1} = x + 1 \end{aligned}$$

$$\begin{aligned} s_2(x) &= f(x_1) \left(\frac{x - x_2}{x_1 - x_2} \right) + f(x_2) \left(\frac{x - x_1}{x_2 - x_1} \right) = f(0) \left(\frac{x - 1}{0 - 1} \right) + f(1) \left(\frac{x - 0}{1 - 0} \right) \\ &= (1) \frac{x-1}{-1} + (3) \frac{x}{1} = 1 + 2x \end{aligned}$$

$$\therefore S(x) = \begin{cases} 1 + x, & x \in [-1, 0] \\ 1 + 2x, & x \in [0, 1] \end{cases}$$

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NOTE:

A drawback for linear splines is that $S(x)$ is generally discontinuous at each interior nodes x_i .

For example, the derivative of $S(x)$ in Example 4.3.1 is discontinuous at $x = 0$.

4.3.2. Quadratic Splines

Suppose we want to join the set of data

$$(x_0, f(x_0)), (x_1, f(x_1)), \dots, (x_n, f(x_n)), \quad \text{where } a = x_0 < x_1 < \dots < x_n = b,$$

by piecewise-quadratic polynomials. Then,

$$S(x) = \begin{cases} s_1(x) = a_0 + b_0x + c_0x^2, & x \in [x_0, x_1] \\ s_2(x) = a_1 + b_1x + c_1x^2, & x \in [x_1, x_2] \\ \vdots \\ s_n(x) = a_{n-1} + b_{n-1}x + c_{n-1}x^2, & x \in [x_{n-1}, x_n] \end{cases}$$

To ensure that $S(x)$ interpolates the data, we set

$$\begin{aligned} s_i(x_{i-1}) &= f(x_{i-1}), \quad i = 1, 2, \dots, n \\ s_i(x_i) &= f(x_i). \end{aligned}$$

To ensure that $S(x)$ is continuous and has continuous first-order derivative everywhere in $[a, b]$, we set

$$s'_i(x_i) = s'_{i+1}(x_i), \quad i = 1, 2, \dots, n-1.$$

Since each s_i has 3 unknown constants, $S(x)$ will give a total of $3n$ unknown coefficients.

The condition $s'_i(x_i) = s'_{i+1}(x_i)$ imposes $n-1$ linear conditions and interpolation imposes $2n$ linear conditions giving a total of $3n-1$ imposed linear conditions. This means that the conditions will give a system of $3n-1$ linear equations in $3n$ unknown coefficients, which may give infinite-many solutions. To get a unique solution, we need to impose another condition. The problem is to determine what additional condition to impose to make the solution unique, for example, $f'(x_0) = S'(x_0)$ or $f'(x_n) = S'(x_n)$. One way to avoid this problem is to set the second derivative of s_1 to zero, i.e. $c_0 = 0$.

Example 4.3.2

Construct a quadratic spline interpolating $(-1, 0)$, $(0, 1)$ and $(1, 3)$.

Solution:

Since the interval $[-1, 1]$ has been divided into three intervals, we must have

$$S(x) = \begin{cases} s_1(x) = a_0 + b_0x, & x \in [-1, 0] \\ s_2(x) = a_1 + b_1x + c_1x^2, & x \in [0, 1] \end{cases}$$

To ensure that $S(x)$ interpolates the data, we have that

$$\begin{aligned} s_1(x_0) &= f(x_0), \quad s_1(x_1) = s_2(x_1) = f(x_1) \quad \text{and} \quad s_2(x_2) = f(x_2) \\ \Rightarrow s_1(-1) &= f(-1) \Leftrightarrow a_0 + b_0(-1) = 0 \Rightarrow a_0 = b_0 \end{aligned}$$

$$s_1(0) = s_2(0) \Leftrightarrow a_0 + b_0(0) = a_1 + b_1(0) + c_1(0^2) \Rightarrow a_0 = a_1 \text{ and } s_1(0) = f(0) \Rightarrow a_0 = a_1 = 1$$

$$s_2(1) = f(1) \Leftrightarrow a_1 + b_1(1) + c_1(1^2) = 3 \Rightarrow b_1 + c_1 = 2$$

To ensure that $S(x)$ is continuous and has continuous first-order derivative everywhere in $[-1,1]$, we have that

$$s_1'(x_1) = s_2'(x_1) \Leftrightarrow b_0 = b_1 + c_1 x_1 \Rightarrow b_0 = b_1 + c_1(0)$$

Since $b_0 = 1$, we get $b_0 = b_1 = 1$ and $b_1 + c_1 = 2 \Rightarrow c_1 = 1$.

$$\therefore S(x) = \begin{cases} 1+x, & x \in [-1,0] \\ 1+x+x^2, & x \in [0,1] \end{cases}$$

Check that $S(x)$ interpolates the data and that $S \in C^1[-1,1]$.

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4.3.3. Cubic Splines

We consider a piecewise-polynomial approximation that uses cubic polynomials between each successive pair of nodes.

Definition 4.3.1

Given a function f defined on $[a,b]$ and a set of nodes $a = x_0 < x_1 < \dots < x_n = b$, a cubic spline interpolant S for f is a function that satisfies the following conditions:

1. $S(x)$ is a cubic polynomial, denoted $S_j(x)$, on the interval $[x_j, x_{j+1}]$ for each $j = 0, 1, 2, \dots, n-1$
2. $S_j(x_j) = f(x_j)$ and $S_j(x_{j+1}) = f(x_{j+1})$ for each $j = 0, 1, 2, \dots, n-1$.
3. $S_{j+1}(x_{j+1}) = S_j(x_{j+1})$, for each $j = 0, 1, 2, \dots, n-2$
4. $S'_{j+1}(x_{j+1}) = S'_j(x_{j+1})$, for each $j = 0, 1, 2, \dots, n-2$
5. $S''_{j+1}(x_{j+1}) = S''_j(x_{j+1})$, for each $j = 0, 1, 2, \dots, n-2$
6. One of the following sets of boundary conditions is satisfied:
 - (i) $S''(x_0) = S''(x_n) = 0$ (Natural (or free) boundary)
 - (ii) $S'(x_0) = f'(x_0)$ and $S'(x_n) = f'(x_n)$ (Clamped boundary)

When natural boundary conditions occur, the spline is called Natural Spline and when clamped boundary conditions occur, we have Clamped Spline.

Using Definition 4.3.1, we will construct cubic splines of the form

$$S_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$$

for each $j = 0, 1, 2, \dots, n-1$.

Example 4.3.3

1. Construct a natural cubic spline that passes through the points (1,2), (2,3) and (3,5).
2. Construct a clamped cubic spline that passes through the points (1,2), (2,3) (3,5) and has $S'(1) = 2$ and $S'(3) = 1$.

Solutions:

From the given data, we have that $x_0 = 1$, $x_1 = 2$, $x_2 = 3$, $S_0(x) \in [1, 2]$ and $S_1(x) \in [2, 3]$ where

$$S_0(x) = a_0 + b_0(x-1) + c_0(x-1)^2 + d_0(x-1)^3 \text{ and } S_1(x) = a_1 + b_1(x-2) + c_1(x-2)^2 + d_1(x-2)^3$$

so that

$$S(x) = \begin{cases} S_0(x), & x \in [1, 2] \\ S_1(x), & x \in [2, 3] \end{cases}$$

$$1. \quad S(1) = f(1) = 2 \Rightarrow S_0(1) = a_0 = 2$$

$$S(2) = f(2) = 3 \Rightarrow S_0(2) = a_0 + b_0 + c_0 + d_0 = 3 \Rightarrow b_0 + c_0 + d_0 = 1. \quad (\text{i})$$

$$\text{Also, } S_1(2) = 3 \Rightarrow a_1 = 3$$

$$S(3) = f(3) = 5 \Rightarrow S_1(3) = S_1(x) = a_1 + b_1 + c_1 + d_1 = 5 \Rightarrow b_1 + c_1 + d_1 = 2 \quad (\text{ii})$$

$$\begin{aligned} S_0'(2) = S_1'(2) &\Leftrightarrow b_0 + 2c_0(2-1) + 3d_0(2-1) = b_1 + 2c_1(2-2) + 3d_1(2-2) \\ &\Rightarrow b_0 - b_1 + 2c_0 + 3d_0 = 0 \end{aligned} \quad (\text{iii})$$

$$\begin{aligned} S_0''(2) = S_1''(2) &\Leftrightarrow 2c_0 + 6d_0(2-1) = 2c_1 + 6d_1(2-2) \\ &\Rightarrow c_0 - c_1 + 3d_0 = 0 \end{aligned} \quad (\text{iv})$$

Using natural conditions, we get

$$\begin{aligned} S''(x_0) = S''(x_n) = 0 &\Rightarrow S''(1) = S''(3) = 0 \\ &\Rightarrow 2c_0 + 6d_0(1-1) = 0 \Rightarrow c_0 = 0 \end{aligned}$$

$$\text{And } 2c_1 + 6d_1(3-2) = 0 \Rightarrow c_1 + 3d_1 = 0 \quad (\text{v})$$

Solving the system formed by equations (i) - (v), we get

$$\begin{aligned} b_0 + d_0 &= 1 \\ b_1 + c_1 + d_1 &= 2 \\ b_0 - b_1 + 3d_0 &= 0 \\ -c_1 + 3d_0 &= 0 \\ c_1 + 3d_1 &= 0 \end{aligned} \Rightarrow \begin{pmatrix} 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & -1 & 0 & 3 & 0 \\ 0 & 0 & -1 & 3 & 0 \\ 0 & 0 & 1 & 0 & 3 \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ c_1 \\ d_0 \\ d_1 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & 1 & 0 & | & 1 \\ 0 & 1 & 1 & 0 & 1 & | & 2 \\ 1 & -1 & 0 & 3 & 0 & | & 0 \\ 0 & 0 & -1 & 3 & 0 & | & 0 \\ 0 & 0 & 1 & 0 & 3 & | & 0 \end{pmatrix} \xrightarrow[r_5 \rightarrow r_4 + r_5]{r_3 \rightarrow r_3 - r_1} \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & | & 1 \\ 0 & 1 & 1 & 0 & 1 & | & 2 \\ 0 & -1 & 0 & 2 & 0 & | & -1 \\ 0 & 0 & -1 & 3 & 0 & | & 0 \\ 0 & 0 & 0 & 3 & 3 & | & 0 \end{pmatrix} \xrightarrow[r_5 \rightarrow \frac{1}{3}r_5]{r_3 \rightarrow r_2 + r_3} \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & | & 1 \\ 0 & 1 & 1 & 0 & 1 & | & 2 \\ 0 & 0 & 1 & 2 & 1 & | & 1 \\ 0 & 0 & -1 & 3 & 0 & | & 0 \\ 0 & 0 & 0 & 1 & 1 & | & 0 \end{pmatrix}$$

$$\xrightarrow{r_4 \rightarrow r_3 + r_4} \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & | & 1 \\ 0 & 1 & 1 & 0 & 1 & | & 2 \\ 0 & 0 & 1 & 2 & 1 & | & 1 \\ 0 & 0 & 0 & 5 & 1 & | & 1 \\ 0 & 0 & 0 & 1 & 1 & | & 0 \end{pmatrix} \xrightarrow{r_5 \rightarrow r_5 - \frac{1}{5}r_4} \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & | & 1 \\ 0 & 1 & 1 & 0 & 1 & | & 2 \\ 0 & 0 & 1 & 2 & 1 & | & 1 \\ 0 & 0 & 0 & 5 & 1 & | & 1 \\ 0 & 0 & 0 & 0 & \frac{4}{5} & | & -\frac{1}{5} \end{pmatrix}$$

$$\therefore \frac{4}{5}d_1 = -\frac{1}{5} \Rightarrow d_1 = -\frac{1}{4}$$

$$5d_0 + d_1 = 1 \Rightarrow d_0 = \frac{1}{4}$$

$$c_1 + 2d_0 + d_1 = 1 \Rightarrow c_1 = \frac{3}{4}$$

$$b_1 + c_1 + d_1 = 2 \Rightarrow b_1 = \frac{3}{2}$$

$$b_0 + d_0 = 1 \Rightarrow b_0 = \frac{3}{4}$$

$$\therefore S(x) = \begin{cases} 2 + \frac{3}{4}(x-1) + \frac{1}{4}(x-1)^3, & x \in [1, 2] \\ 3 + \frac{3}{2}(x-2) + \frac{3}{4}(x-2)^2 - \frac{1}{4}(x-2)^3, & x \in [2, 3] \end{cases}$$

2. The first five conditions are as in part 1, i.e.

$$S_0(1) = a_0 = 2$$

$$S_0(2) = S_1(2) = 3 \Rightarrow a_0 + b_0 + c_0 + d_0 = 3 \Rightarrow b_0 + c_0 + d_0 = 1 \quad \text{and} \quad S_1(2) = 3 \Rightarrow a_1 = 3$$

$$S_1(3) = 5 \Rightarrow a_1 + b_1 + c_1 + d_1 = 5 \Rightarrow b_1 + c_1 + d_1 = 2$$

$$S_0'(2) = S_1'(2) \Leftrightarrow b_0 - b_1 + 2c_0 + 3d_0 = 0 \quad \text{and} \quad S_0''(2) = S_1''(2) \Leftrightarrow c_0 - c_1 + 3d_0 = 0$$

Using clamped condition, we get

$$S'(x_0) = f'(x_0) \Leftrightarrow S'(1) = 2 \Rightarrow b_0 + 2c_0(1-1) + 3d_0(1-1) = 2 \Rightarrow b_0 = 2$$

$$\text{And } S'(x_n) = f'(x_n) \Leftrightarrow S'(3) = 1 \Rightarrow b_1 + 2c_1(3-2) + 3d_1(3-2) = 1 \Rightarrow b_1 + 2c_1 + 3d_1 = 1.$$

Thus,

$$\begin{pmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ -1 & 2 & 0 & 3 & 0 \\ 0 & 1 & -1 & 3 & 0 \\ 1 & 0 & 2 & 0 & 3 \end{pmatrix} \begin{pmatrix} b_1 \\ c_0 \\ c_1 \\ d_0 \\ d_1 \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \\ -2 \\ 0 \\ 1 \end{pmatrix} \Rightarrow \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & | & -1 \\ 1 & 0 & 1 & 0 & 1 & | & 2 \\ -1 & 2 & 0 & 3 & 0 & | & -2 \\ 0 & 1 & -1 & 3 & 0 & | & 0 \\ 1 & 0 & 2 & 0 & 3 & | & 1 \end{pmatrix} \xrightarrow{r_1 \leftrightarrow r_2} \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & | & 2 \\ 0 & 1 & 0 & 1 & 0 & | & -1 \\ -1 & 2 & 0 & 3 & 0 & | & -2 \\ 0 & 1 & -1 & 3 & 0 & | & 0 \\ 1 & 0 & 2 & 0 & 3 & | & 1 \end{pmatrix}$$

$$\begin{array}{l} r_3 \rightarrow r_3 + r_1 \\ r_5 \rightarrow r_5 - r_1 \\ r_4 \rightarrow r_2 - r_4 \end{array} \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & | & 2 \\ 0 & 1 & 0 & 1 & 0 & | & -1 \\ 0 & 2 & 1 & 3 & 1 & | & 0 \\ 0 & 0 & 1 & -2 & 0 & | & -1 \\ 0 & 0 & 1 & 0 & 2 & | & -1 \end{pmatrix} \xrightarrow{\begin{array}{l} r_3 \rightarrow r_3 - 2r_2 \\ r_5 \rightarrow r_5 - r_4 \end{array}} \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & | & 2 \\ 0 & 1 & 0 & 1 & 0 & | & -1 \\ 0 & 0 & 1 & 1 & 1 & | & 2 \\ 0 & 0 & 1 & -2 & 0 & | & -1 \\ 0 & 0 & 0 & 2 & 2 & | & 0 \end{pmatrix} \xrightarrow{\begin{array}{l} r_4 \rightarrow r_3 - r_4 \\ r_5 \rightarrow \frac{1}{2}r_5 \end{array}}$$

$$\begin{pmatrix} 1 & 0 & 1 & 0 & 1 & | & 2 \\ 0 & 1 & 0 & 1 & 0 & | & -1 \\ 0 & 0 & 1 & 1 & 1 & | & 2 \\ 0 & 0 & 0 & 3 & 1 & | & 3 \\ 0 & 0 & 0 & 1 & 1 & | & 0 \end{pmatrix} \xrightarrow{r_5 \rightarrow r_5 - \frac{1}{3}r_4} \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & | & 2 \\ 0 & 1 & 0 & 1 & 0 & | & -1 \\ 0 & 0 & 1 & 1 & 1 & | & 2 \\ 0 & 0 & 0 & 3 & 1 & | & 3 \\ 0 & 0 & 0 & 0 & \frac{2}{3} & | & -1 \end{pmatrix}$$

$$\therefore \frac{2}{3}d_1 = -1 \Rightarrow d_1 = -\frac{3}{2}$$

$$3d_0 + d_1 = 3 \Rightarrow d_0 = \frac{3}{2}$$

$$c_1 + d_0 + d_1 = 2 \Rightarrow c_1 = 2$$

$$c_0 + d_0 = -1 \Rightarrow c_0 = -\frac{5}{2}$$

$$b_1 + c_1 + d_1 = 2 \Rightarrow b_1 = \frac{3}{2}$$

$$\therefore S(x) = \begin{cases} 2 + 2(x-1) - \frac{5}{2}(x-1)^2 + \frac{3}{2}(x-1)^3, & x \in [1, 2] \\ 3 + \frac{3}{2}(x-2) + 2(x-2)^2 - \frac{3}{2}(x-2)^3, & x \in [2, 3] \end{cases}$$

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4.4. LEAST-SQUARES APPROXIMATION

Suppose that a mathematical equation is to be fitted to experimental data by plotting the data on a graph paper and then passing a line through the data points. The method of least squares endeavours to determine the best approximating line by minimising the sum of the squares of error, i.e. if (x_i, y_i) , $i = 1, 2, 3, \dots, n$ are data points and $Y = f(x)$ is the curve to be fitted to this data, then the error is

$$e_i = y_i - f(x_i)$$

and the sum of the squares of the errors is

$$S = [y_1 - f(x_1)]^2 + [y_2 - f(x_2)]^2 + \dots + [y_n - f(x_n)]^2. \quad (4.4)$$

Then the method of least-squares involves minimising S .

Straight line: Let $Y = a_0 + a_1x$ be the straight line to be fitted to the given data. Then,

$$S = [y_1 - (a_0 + a_1x_1)]^2 + [y_2 - (a_0 + a_1x_2)]^2 + \dots + [y_n - (a_0 + a_1x_n)]^2$$

and minimising S implies that

$$\begin{aligned} \frac{\partial S}{\partial a_0} = 0 &\Rightarrow -2[y_1 - (a_0 + a_1x_1)] - 2[y_2 - (a_0 + a_1x_2)] - \dots - 2[y_n - (a_0 + a_1x_n)] = 0 \\ &\Rightarrow -2 \sum_{i=1}^n [y_i - (a_0 + a_1x_i)] = 0 \end{aligned} \quad (4.5)$$

and

$$\begin{aligned} \frac{\partial S}{\partial a_1} = 0 &\Rightarrow -2x_1[y_1 - (a_0 + a_1x_1)] - 2x_2[y_2 - (a_0 + a_1x_2)] - \dots - 2x_n[y_n - (a_0 + a_1x_n)] = 0 \\ &\Rightarrow -2 \sum_{i=1}^n x_i [y_i - (a_0 + a_1x_i)] = 0. \end{aligned} \quad (4.6)$$

Simplifying (4.5) and (4.6) leads to what are known as normal equations:

$$\begin{aligned} -2 \sum_{i=1}^n [y_i - (a_0 + a_1x_i)] = 0 &\Rightarrow \sum_{i=1}^n y_i - \sum_{i=1}^n a_0 - a_1 \sum_{i=1}^n x_i = 0 \\ &\Rightarrow \sum_{i=1}^n y_i - na_0 - a_1 \sum_{i=1}^n x_i = 0 \end{aligned} \quad (4.7)$$

and

$$\begin{aligned}
 -2 \sum_{i=1}^n x_i [y_i - (a_0 + a_1 x_i)] &= 0 \Rightarrow \sum_{i=1}^n x_i y_i - a_0 \sum_{i=1}^n x_i - a_1 \sum_{i=1}^n x_i^2 = 0 \\
 \Rightarrow \sum_{i=1}^n x_i y_i &= a_0 \sum_{i=1}^n x_i + a_1 \sum_{i=1}^n x_i^2
 \end{aligned} \tag{4.8}$$

Solving (4.7) and (4.8) simultaneously, we get

$$\begin{aligned}
 a_1 &= \frac{n \sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right)}{n \left(\sum_{i=1}^n x_i^2 \right) - \left(\sum_{i=1}^n x_i \right)^2} \\
 a_0 &= \frac{\left(\sum_{i=1}^n x_i^2 \right) \left(\sum_{i=1}^n y_i \right) - \left(\sum_{i=1}^n x_i y_i \right) \left(\sum_{i=1}^n x_i \right)}{n \left(\sum_{i=1}^n x_i^2 \right) - \left(\sum_{i=1}^n x_i \right)^2}.
 \end{aligned}$$

Letting $\bar{x} = \frac{\sum_{i=1}^n x_i}{n}$ and $\bar{y} = \frac{\sum_{i=1}^n y_i}{n}$, we can rewrite the formulas for a_0 and a_1 as

$$\begin{aligned}
 a_1 &= \frac{\sum_{i=1}^n x_i y_i - n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - n \bar{x}^2} \\
 a_0 &= \frac{\bar{y} \left(\sum_{i=1}^n x_i^2 \right) - \bar{x} \left(\sum_{i=1}^n x_i y_i \right)}{\sum_{i=1}^n x_i^2 - n \bar{x}^2}.
 \end{aligned}$$

Clearly, $\frac{\partial^2 S}{\partial a_0^2} > 0$ and $\frac{\partial^2 S}{\partial a_1^2} > 0$ showing that these values of a_0 and a_1 provide a minimum of S .

Example 4.4.1

The table below gives the temperature T (in $^{\circ}C$) and length l (in mm) of a heated rod. If $l = a + bT$, find the best values of a and b .

T	20	30	40	50	60	70
l	800.3	800.4	800.6	800.7	800.9	801.0

Solution:

	T	l	T^2	Tl
	20	800.3	400	16006
	30	800.4	900	24012
	40	800.6	1600	32024
	50	800.7	2500	40035
	60	800.9	3600	48054
	70	801.0	4900	56070
Sum	270	4803.9	13900	216201

$$\therefore n = 6, \sum T = 270, \sum l = 4803.9, \sum T^2 = 13900, \sum Tl = 216201$$

$$b = \frac{n \sum Tl - \left(\sum T \right) \left(\sum l \right)}{n \left(\sum T^2 \right) - \left(\sum T \right)^2} = \frac{6(216201) - (270)(4803.9)}{6(13900) - (270)^2} = 0.014571428 \approx 0.0146$$

$$a = \frac{\left(\sum T^2 \right) \left(\sum l \right) - \left(\sum Tl \right) \left(\sum T \right)}{n \left(\sum T^2 \right) - \left(\sum T \right)^2} = \frac{(13900)(4803.9) - (216201)(270)}{6(13900) - (270)^2} = 799.9942857 \approx 800$$

$$\therefore l = 800 + 0.0146T$$

Δ

Polynomial of the k^{th} degree: Let $Y = a_0 + a_1x + a_2x^2 + \dots + a_kx^k$ be the polynomial of the k^{th} -order to be fitted to the data $(x_i, y_i), i = 1, 2, \dots, n$. Then, we minimise

$$S = [y_1 - (a_0 + a_1x_1 + a_2x_1^2 + \dots + a_kx_1^k)]^2 + [y_2 - (a_0 + a_1x_2 + a_2x_2^2 + \dots + a_kx_2^k)]^2 + \dots + [y_n - (a_0 + a_1x_n + a_2x_n^2 + \dots + a_kx_n^k)]^2$$

by setting $\frac{\partial S}{\partial a_i} = 0$, for $i = 0, 1, 2, \dots, k$. This leads to the following $k + 1$ normal equations in

$k + 1$ unknowns:

$$\begin{aligned}
na_0 + a_1 \sum_{i=1}^n x_i + a_2 \sum_{i=1}^n x_i^2 + \dots + a_k \sum_{i=1}^n x_i^k &= \sum_{i=1}^n y_i \\
a_0 \sum_{i=1}^n x_i + a_1 \sum_{i=1}^n x_i^2 + a_2 \sum_{i=1}^n x_i^3 + \dots + a_k \sum_{i=1}^n x_i^{k+1} &= \sum_{i=1}^n x_i y_i \\
\vdots & \\
a_0 \sum_{i=1}^n x_i^k + a_1 \sum_{i=1}^n x_i^{k+1} + a_2 \sum_{i=1}^n x_i^{k+2} + \dots + a_k \sum_{i=1}^n x_i^{2k} &= \sum_{i=1}^n x_i^k y_i
\end{aligned}$$

Example 4.4.2

Fit a polynomial of the second degree to the data points given below:

x	0	1.0	2.0
y	1.0	6.0	17.0

Solution:

Let $Y = a_0 + a_1x + a_2x^2$, where $n = 3$ and $k = 2$. The normal equations are

$$\begin{aligned}
na_0 + a_1 \sum_{i=1}^n x_i + a_2 \sum_{i=1}^n x_i^2 &= \sum_{i=1}^n y_i & 3a_0 + a_1 \sum_{i=1}^n x_i + a_2 \sum_{i=1}^n x_i^2 &= \sum_{i=1}^n y_i \\
a_0 \sum_{i=1}^n x_i + a_1 \sum_{i=1}^n x_i^2 + a_2 \sum_{i=1}^n x_i^3 &= \sum_{i=1}^n x_i y_i & \Rightarrow a_0 \sum_{i=1}^n x_i + a_1 \sum_{i=1}^n x_i^2 + a_2 \sum_{i=1}^n x_i^3 &= \sum_{i=1}^n x_i y_i \\
a_0 \sum_{i=1}^n x_i^k + a_1 \sum_{i=1}^n x_i^{k+1} + a_2 \sum_{i=1}^n x_i^{2k} &= \sum_{i=1}^n x_i^k y_i & a_0 \sum_{i=1}^n x_i^2 + a_1 \sum_{i=1}^n x_i^3 + a_2 \sum_{i=1}^n x_i^4 &= \sum_{i=1}^n x_i^2 y_i
\end{aligned}$$

x	y	x^2	x^3	x^4	xy	x^2y
0	1	0	0	0	0	0
1	6	1	1	1	6	6
2	17	4	8	16	34	68

$$\sum: \quad 3 \quad 24 \quad 5 \quad 9 \quad 17 \quad 40 \quad 74$$

Using normal equations, we get a system of linear equations

$$\begin{aligned}
3a_0 + 3a_1 + 5a_2 &= 24 \\
3a_0 + 5a_1 + 9a_2 &= 40 \\
5a_0 + 9a_1 + 17a_2 &= 74
\end{aligned}$$

whose solution is $a_0 = 1$, $a_1 = 2$ and $a_2 = 3$.

$$\therefore Y = 1 + 2x + 3x^2$$

Δ

Exponential function: Let the curve $y = a_0 e^{a_1 x}$ be fitted to the data (x_i, y_i) , $i = 1, 2, \dots, n$.

Then, taking natural logarithms on both sides, we get

$$\ln y = \ln(a_0 e^{a_1 x}) = \ln a_0 + a_1 x,$$

which can be written as

$$Y = A_0 + A_1 x,$$

where $Y = \ln y$, $A_0 = \ln a_0$, $A_1 = a_1$ and this can be treated as a straight line problem.

Example 4.4.3

Fit an exponential function to the data given in the table below:

x	1.00	1.25	1.50	1.75	2.00
y	5.10	5.79	6.53	7.45	8.46

Solution:

We transform $y = a_0 e^{a_1 x}$ into $Y = A_0 + A_1 x$, where $Y = \ln y$, $A_0 = \ln a_0$, $A_1 = a_1$ and $n = 5$.

$$5A_0 + A_1 \sum x_i = \sum Y_i = \sum \ln y_i$$

$$A_0 \sum x_i + A_1 \sum x_i^2 = \sum x_i Y_i = \sum x_i \ln y_i$$

x	y	$\ln y$	x^2	$x \ln y$
1.00	5.10	1.629	1.00	1.629
1.25	5.79	1.756	1.5625	2.195
1.50	6.53	1.876	2.2500	2.814
1.75	7.45	2.008	3.0625	3.514
2.00	8.46	2.135	4.0000	4.270
Σ :	7.5	9.404	11.875	14.422

$$\begin{aligned} 5A_0 + A_1 \sum x_i &= \sum \ln y_i \\ A_0 \sum x_i + A_1 \sum x_i^2 &= \sum x_i \ln y_i \end{aligned} \Rightarrow \begin{aligned} 5A_0 + 7.5A_1 &= 9.404 \\ 7.5A_0 + 11.875A_1 &= 14.422 \end{aligned}$$

$$A_1 = \frac{9.404 - 5A_0}{7.5} \Rightarrow 7.5A_0 + 11.875\left(\frac{9.404 - 5A_0}{7.5}\right) = 14.422 \Rightarrow A_0 = 1.1224$$

Since $A_0 = \ln a_0$, we have that $a_0 = e^{1.1224} = 3.072$

$$\Rightarrow A_1 = a_1 = \frac{9.404 - 5(1.1224)}{7.5} = 0.5056$$

$$\therefore y = 3.072e^{0.5056x}$$

Δ

4.4.1. Weighted Least-Squares Approximation

If the given data is not of equal quality, the fit by minimising the sum of squares of the errors may not be very accurate. To improve the fit, a more general approach is to minimise the weighted sum of squares of the errors taken over all data points

$$\begin{aligned} S &= w_1[y_1 - f(x_1)]^2 + w_2[y_2 - f(x_2)]^2 + \dots + w_n[y_n - f(x_n)]^2 \\ &= w_1e_1^2 + w_2e_2^2 + \dots + w_ne_n^2. \end{aligned}$$

The w_i 's are prescribed positive numbers and are called weights. A weight is prescribed according to the relative accuracy of a data point. If all the data points are accurate, we set $w_i = 1$ for all i .

Example 4.4.4

In Example 4.4.1 we got the linear fit $l = 800 + 0.0146T$. Suppose that the point (60, 800.9) is known to be more reliable than the others. Then we prescribe a weight (say 10) corresponding to this point only and set $w_i = 1$, for all other points so that

$$\begin{aligned} a_0 \sum_{i=1}^n w_i + a_1 \sum_{i=1}^n w_i T_i &= \sum_{i=1}^n w_i l_i \\ a_0 \sum_{i=1}^n w_i T_i + a_1 \sum_{i=1}^n w_i T_i^2 &= \sum_{i=1}^n w_i T_i l_i \end{aligned}$$

T	l	w	T^2	wT	wl	Tl	wT^2	wTl
20	800.3	1	400	20	800.3	16006	400	16006
30	800.4	1	900	30	800.4	24012	900	24012
40	800.6	1	1600	40	800.6	32024	1600	32024
50	800.7	1	2500	50	800.7	40035	2500	40035
60	800.9	10	3600	600	8009.0	48054	36000	480540
70	801.0	1	4900	70	801.0	56070	4900	56070

$$\sum: \quad 270 \quad 4803.9 \quad 15 \quad 13900 \quad 810 \quad 12012 \quad 216201 \quad 46300 \quad 648687$$

$$\begin{aligned} a_0 \sum_{i=1}^n w_i + a_1 \sum_{i=1}^n w_i T_i &= \sum_{i=1}^n w_i l_i \\ a_0 \sum_{i=1}^n w_i T_i + a_1 \sum_{i=1}^n w_i T_i^2 &= \sum_{i=1}^n w_i T_i l_i \end{aligned} \Rightarrow \begin{aligned} 15a_0 + 810a_1 &= 12012 \\ 810a_0 + 46300a_1 &= 648687 \end{aligned}$$

$$a_1 = \frac{12012 - 15a_0}{810}$$

$$\Rightarrow 810a_0 + 46300 \left(\frac{12012 - 15a_0}{810} \right) = 648687 \Rightarrow a_0 = 800$$

$$\Rightarrow a_1 = \frac{12012 - 15(800)}{810} = 0.0148$$

$$\therefore l = 800 + 0.0148T$$

Note that the first fit gives

$$l(60) = 800 + 0.0146(60) = 800.876$$

and the weighted fit gives

$$l(60) = 800 + 0.0148(60) = 800.888$$

Note that the approximation becomes better when the weight is increased.

Δ

4.4.2. Least-Squares for Continuous Functions

We discuss the least squares approximation of a continuous function on an interval $[a, b]$.

Let $Y(x) = a_0 + a_1x + \dots + a_nx^n$ be chosen to minimise

$$S = \int_a^b w(x) \left[y(x) - (a_0 + a_1x + \dots + a_nx^n) \right]^2 dx$$

The necessary conditions for a minimum yield

$$\begin{aligned} -2 \int_a^b w(x) \left[y(x) - (a_0 + a_1 x + \dots + a_n x^n) \right] dx &= 0 \\ -2 \int_a^b x.w(x) \left[y(x) - (a_0 + a_1 x + \dots + a_n x^n) \right] dx &= 0 \\ \vdots \\ -2 \int_a^b x^n w(x) \left[y(x) - (a_0 + a_1 x + \dots + a_n x^n) \right] dx &= 0 \end{aligned}$$

Rearrangement of terms gives the following normal equations:

$$\begin{aligned} a_0 \int_a^b w(x) dx + a_1 \int_a^b x.w(x) dx + a_2 \int_a^b x^2.w(x) dx + \dots + a_n \int_a^b x^n.w(x) dx &= \int_a^b w(x) y(x) dx \\ a_0 \int_a^b x.w(x) dx + a_1 \int_a^b x^2.w(x) dx + a_2 \int_a^b x^3.w(x) dx + \dots + a_n \int_a^b x^{n+1}.w(x) dx &= \int_a^b x.w(x) y(x) dx \\ \vdots \\ a_0 \int_a^b x^n.w(x) dx + a_1 \int_a^b x^{n+1}.w(x) dx + a_2 \int_a^b x^{n+2}.w(x) dx + \dots + a_n \int_a^b x^{2n}.w(x) dx &= \int_a^b x^n.w(x) y(x) dx \end{aligned}$$

Example 4.4.5

Find the least-squares approximating polynomial of degree two for the function $f(x) = \sin \pi x$ on the interval $[0, 1]$ with respect to the weight function $w(x) = 1$.

Solution:

The normal equations for $Y(x) = a_0 + a_1 x + a_2 x^2$ are

$$\begin{aligned} a_0 \int_0^1 dx + a_1 \int_0^1 x dx + a_2 \int_0^1 x^2 dx &= \int_0^1 \sin \pi x dx & a_0 + \frac{1}{2} a_1 + \frac{1}{3} a_2 &= \frac{2}{\pi} \\ a_0 \int_0^1 x dx + a_1 \int_0^1 x^2 dx + a_2 \int_0^1 x^3 dx &= \int_0^1 x \sin \pi x dx & \Rightarrow \frac{1}{2} a_0 + \frac{1}{3} a_1 + \frac{1}{4} a_2 &= \frac{2}{\pi} \\ a_0 \int_0^1 x^2 dx + a_1 \int_0^1 x^3 dx + a_2 \int_0^1 x^4 dx &= \int_0^1 x^2 \sin \pi x dx & \frac{1}{3} a_0 + \frac{1}{4} a_1 + \frac{1}{5} a_2 &= \frac{\pi^2 - 4}{\pi^3} \end{aligned}$$

Solving this system gives

$$a_0 = \frac{12\pi^2 - 120}{\pi^3} \approx -0.050465$$

$$a_1 = \frac{720 - 60\pi^2}{\pi^3} \approx 4.12251$$

$$a_2 = \frac{60\pi^2 - 720}{\pi^3} \approx -4.12251$$

$$\therefore Y(x) = -0.050465 + 4.12251x - 4.12251x^2$$

Δ

4.5. CHEBYSHEV POLYNOMIALS AND ECONOMISATION OF POWER SERIES

Let f_1, f_2, \dots, f_n be values of the given function and $\phi_1, \phi_2, \dots, \phi_n$ be the corresponding values of the approximating function. Then the error vector e , where the components of e are given by $e_i = f_i - \phi_i$. The approximation may be chosen using least-squares method or may be chosen in such a way that the maximum component of e is minimised. The later method leads to Chebyshev polynomials.

4.5.1. Chebyshev Polynomials

The Chebyshev polynomial of degree n over the interval $[-1, 1]$ is defined by

$$T_n(x) = \cos(n \cos^{-1} x)$$

from which we get the relation

$$T_n(x) = T_{-n}(x).$$

Letting $\cos^{-1} x = \theta$ implies that $\cos \theta = x$ so that

$$T_n(x) = \cos n\theta.$$

Hence, $T_0(x) = 1$ and $T_1(x) = x$. Using the trigonometric identity

$$\cos[(n-1)\theta] + \cos[(n+1)\theta] = 2\cos(n\theta)\cos\theta$$

we have that

$$\begin{aligned} T_{n-1}(x) + T_{n+1}(x) &= 2xT_n(x) \\ \Rightarrow T_{n+1}(x) &= 2xT_n(x) - T_{n-1}(x) \end{aligned}$$

which is the recurrence relation that can be used to complete successively all $T_n(x)$ since we know $T_0(x)$ and $T_1(x)$.

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_2(x) = 2xT_1(x) - T_0(x) = 2x^2 - 1$$

$$T_3(x) = 2xT_2(x) - T_1(x) = 2x(2x^2 - 1) - x = 4x^3 - 3x$$

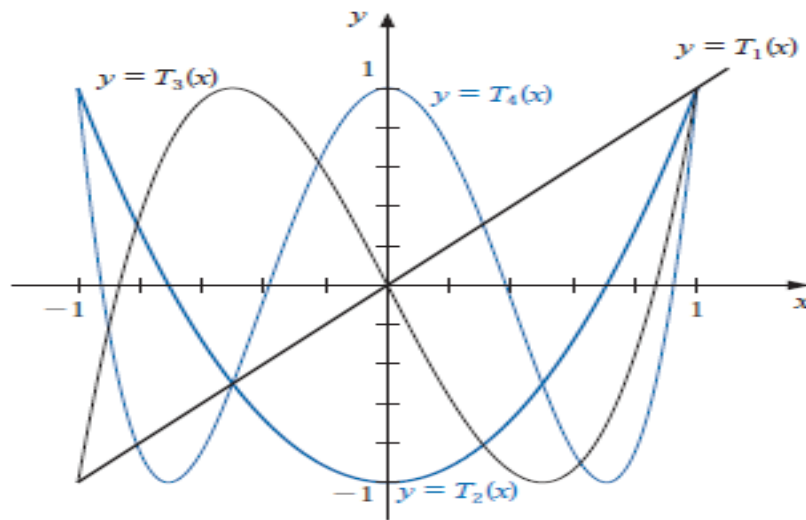
$$T_4(x) = 8x^4 - 8x^2 + 1$$

$$T_5(x) = 16x^5 - 20x^3 + 5x$$

$$T_6(x) = 32x^6 - 48x^4 + 18x^2 - 1$$

$$\vdots$$

The graphs of the first four Chebyshev polynomials are:



Note that the coefficient of x^n in $T_n(x)$ is always 2^{n-1} and $|T_n(x)| \leq 1$, for $n \geq 1$, $-1 \leq x \leq 1$.

If $P_n(x)$ is a monic polynomial such that $P_n(x) = 2^{1-n}T_n(x)$, then $P_n(x)$ has the least upper bound 2^{1-n} since $|T_n(x)| \leq 1$. Thus, in Chebyshev approximation, the maximum error is kept down to a minimum.

It is possible to express powers of x in terms of Chebyshev polynomials. Then

$$1 = T_0(x)$$

$$x = T_1(x)$$

$$x^2 = \frac{1}{2}[T_0(x) + T_2(x)]$$

$$x^3 = \frac{1}{4}[3T_1(x) + T_3(x)]$$

$$x^4 = \frac{1}{8}[3T_0(x) + 4T_2(x) + T_4(x)]$$

$$x^5 = \frac{1}{16}[10T_1(x) + 5T_3(x) + T_5(x)]$$

$$x^6 = \frac{1}{32}[10T_0(x) + 15T_2(x) + 6T_4(x) + T_6(x)]$$

Chebyshev polynomials can be used to reduce the degree of an approximating polynomial with a minimal loss of accuracy. This is known as economisation of power series.

Example 4.5.1

Economise the power series

$$\text{a) } \sin x \approx x - \frac{x^3}{6} + \frac{x^5}{120} - \frac{x^7}{5040}$$

while keeping the error less than 0.005.

$$\text{b) } e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!}$$

while keeping the error less than 0.05.

Solution:

$$\text{a) } \text{Since } \frac{1}{5040} \approx 0.000198... \text{ is the first value which is numerically less than } 0.005,$$

we have that

$$\sin x \approx x - \frac{x^3}{6} + \frac{x^5}{120}.$$

We now express $P_5(x)$ in terms of Chebyshev polynomials.

$$\begin{aligned} P_n(x) &= T_1(x) - \frac{1}{6} \cdot \frac{1}{4} [3T_1(x) + T_3(x)] + \frac{1}{120} \cdot \frac{1}{16} [10T_1(x) + 5T_3(x) + T_5(x)] \\ &= \frac{169}{192} T_1(x) - \frac{5}{128} T_3(x) + \frac{1}{1920} T_5(x). \end{aligned}$$

Since $\frac{1}{1920} \approx 0.00052083 < 0.005$, the economised power series is

$$\begin{aligned} P_3(x) &= \frac{169}{192} T_1(x) - \frac{5}{128} T_3(x) = \frac{169}{192} x - \frac{5}{128} (4x^3 - 3x) \\ &= \frac{383}{384} x - \frac{5}{32} x^3. \end{aligned}$$

b) Remember that the upper bound of the error is

$$|R_4(x)| = \frac{|f^{(5)}(\xi(x))x^5|}{5!} \leq \frac{e}{120} \approx 0.023 \text{ for } -1 \leq x \leq 1.$$

We now express $P_4(x)$ in terms of Chebyshev polynomials.

$$\begin{aligned}
P_4(x) &= T_0(x) + T_1(x) + \frac{1}{4}T_0(x) + \frac{1}{4}T_2(x) + \frac{1}{8}T_1(x) + \frac{1}{24}T_3(x) + \frac{1}{64}T_0(x) + \frac{1}{48}T_2(x) + \frac{1}{192}T_4(x) \\
&= \frac{81}{64}T_0(x) + \frac{9}{8}T_1(x) + \frac{13}{48}T_2(x) + \frac{1}{24}T_3(x) + \frac{1}{192}T_4(x)
\end{aligned}$$

But $\left| \frac{1}{192}T_4(x) \right| \leq \frac{1}{192} = 0.0053$. Thus,

$$|R_4(x)| + \left| \frac{1}{192}T_4(x) \right| \leq 0.023 + 0.0053 = 0.0283 < 0.05.$$

Also,

$$|R_4(x)| + \left| \frac{1}{24}T_3(x) \right| \leq 0.023 + 0.04173 = 0.0647 > 0.05.$$

Therefore,

$$P_3(x) = \frac{81}{64}T_0(x) + \frac{9}{8}T_1(x) + \frac{13}{48}T_2(x) + \frac{1}{24}T_3(x)$$

is the lowest-degree polynomial possible, i.e.

$$P_3(x) = \frac{191}{192} + x + \frac{13}{24}x^2 + \frac{1}{6}x^3$$

Δ

THE END!