Taylor Expansion

One Variable

$f:[a,b] \to R;\ f(x)$, n+1 times differentiable; $f^{(n)}$ continuous.

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!} + \cdots + \frac{f^{(n)}}{n!}(x-a)^n + R_{n+1}(x)$$

$$R_{n+1}(x) = f(x) - \sum_{k=0}^{n} \frac{f^{(k)}}{k!}(x-a)^i = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-a)^{n+1}$$

$$\lim_{x\to a} R_{n+1} = 0$$

Two Variable

U convex open set in R^n; $f: U \to R$; continuous partial derivatives of all orders up to m+1.

$$D_j^l f \coloneqq \frac{\partial^l f}{\partial x_j}, \qquad D_{i_1\dots i_k} f \coloneqq \frac{\partial^k f}{\partial x_{i_1} \dots \partial x_{i_k}}$$

$$f(\boldsymbol{x}) = \sum_{k_1+\dots+k_n \le m} \frac{\left(D_1^{k_1} D_2^{k_2} \dots D_n^{k_n} f\right)(\boldsymbol{x}-\boldsymbol{a})}{k_1!\,k_2! \dots k_n!}(x_1-a_1)^{k_1}(x_2-a_2)^{k_2} \dots (x_n-a_n)^{k_n} + R(\boldsymbol{x})$$

$$f(\boldsymbol{a}+\boldsymbol{x}) = \sum_{k_1+\dots+k_n \le m} \frac{\left(D_1^{k_1} D_2^{k_2} \dots D_n^{k_n} f\right)(\boldsymbol{x})}{k_1!\,k_2! \dots k_n!} {x_1}^{k_1} {x_2}^{k_2} \dots {x_n}^{k_n} + R(\boldsymbol{x})$$

Interpolation and Polynomial approximation

Lagrange Interpolation

$$P_n(x) = \sum_{k=0}^{n} f(x_k) L_k(x), \qquad L_k(x) = \prod_{\substack{i=0 \\ i \ne k}}^{n} \frac{(x-x_i)}{(x_k-x_i)}$$

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

Newton's Divided Difference

$$P_n(x) = f[x_0] + \sum_{k=1}^{n} f[x_0, x_1, \dots x_k](x-x_0)\dots(x-x_{k-1})$$

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

$$f[x_0, x_1, \dots, x_n] = \frac{f^{(n)}(\xi)}{n!}$$

x	$f(x)$	First divided differences	Second divided differences	Third divided differences
x_0	$f[x_0]$			
		$f[x_0,x_1] = \frac{f[x_1]-f[x_0]}{x_1-x_0}$		
x_1	$f[x_1]$		$f[x_0,x_1,x_2] = \frac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0}$	
		$f[x_1,x_2] = \frac{f[x_2]-f[x_1]}{x_2-x_1}$		$f[x_0,x_1,x_2,x_3] = \frac{f[x_1,x_2,x_3]-f[x_0,x_1,x_2]}{x_3-x_0}$
x_2	$f[x_2]$		$f[x_1,x_2,x_3] = \frac{f[x_2,x_3]-f[x_1,x_2]}{x_3-x_1}$	
		$f[x_2,x_3] = \frac{f[x_3]-f[x_2]}{x_3-x_2}$		$f[x_1,x_2,x_3,x_4] = \frac{f[x_2,x_3,x_4]-f[x_1,x_2,x_3]}{x_4-x_1}$
x_3	$f[x_3]$		$f[x_2,x_3,x_4] = \frac{f[x_3,x_4]-f[x_2,x_3]}{x_4-x_2}$	
		$f[x_3,x_4] = \frac{f[x_4]-f[x_3]}{x_4-x_3}$		$f[x_2,x_3,x_4,x_5] = \frac{f[x_3,x_4,x_5]-f[x_2,x_3,x_4]}{x_5-x_2}$
x_4	$f[x_4]$		$f[x_3,x_4,x_5] = \frac{f[x_4,x_5]-f[x_3,x_4]}{x_5-x_3}$	
		$f[x_4,x_5] = \frac{f[x_5]-f[x_4]}{x_5-x_4}$		
x_5	$f[x_5]$			

Chebyshev nodes

$$x_k = \frac{a+b}{2} + \frac{b-a}{2}\cos\left(\frac{2k+1}{2n}\pi\right), \qquad k = 0, \dots, n-1$$

Spline Interpolation

$$S_i(x_{i+1}) = S_{i+1}(x_{i+1}) = f(x_{i+1})$$

$$S_i'(x_{i+1}) = S_{i+1}'(x_{i+1}),\ S_i''(x_{i+1}) = S_{i+1}''(x_{i+1}), \dots,\ S_i^{(k)}(x_{i+1}) = S_{i+1}^{(k)}(x_{i+1})$$

Natural Cubic Spline

$$S''(x_0) = S''(x_n) = 0$$

Clamped Cubic Spline

$$S'(x_0) = f'(x_0), \qquad S'(x_n) = f'(x_n)$$

Linear Spline

$$S_i(x) = f(x_i) + \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}(x - x_i)$$

Numerical Differentiation

(n+1)-Point Formula

$$f'(x) = \sum_{k=0}^{n} f(x_k) L_k'(x) + D_x\left[\frac{(x-x_0)\dots(x-x_n)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) + \frac{(x-x_0)\dots(x-x_n)}{(n+1)!} D_x\left[f^{(n+1)}(\xi(x))\right]$$

$$f'(x_j) = \sum_{k=0}^{n} f(x_k) L_k'(x_j) + \frac{f^{(n+1)}\left(\xi(x_j)\right)}{(n+1)!} \prod_{\substack{k=0 \\ k \ne j}}^{n} (x_j - x_k)$$

Three Point Formulas

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f'''(\xi_0)$$

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f'''(\xi_1)$$

Five Point Formulas

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30} f^{(5)}(\xi)$$

$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] + \frac{h^4}{5} f^{(5)}(\xi)$$

Second Derivative Formula

$$f(x_0+h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$

$$f(x_0-h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4$$

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{1}{24}\left[f^{(4)}(\xi_1) + \frac{1}{24}f^{(4)}(\xi_{-1})\right]h^4$$

$f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$ Intermediate value theorem

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0-h) - 2f(x_0) + f(x_0+h)\right] - \frac{h^2}{12} f^{(4)}(\xi)$$

Other Derivatives

First Derivative	Error
$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4}$	$O(h^4)$

Derivation using Forward Differences

$$P_n(x) = P_n(x_0+sh) = f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta f_0 + \cdots \frac{s(s-1)\dots(s-(n-1))}{n!}\Delta^n f_0 = \sum_{k=0}^{n}\binom{s}{k}\Delta^k f_0$$

$$f'(x) \simeq \frac{dp}{dx} = \frac{dp}{ds}\frac{ds}{dx} = \frac{1}{h}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \cdots + \frac{(-1)^{n-1}}{n}\Delta^n f_0\right]$$

$$E_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)\dots(x-x_n) = f^{(n+1)}(\xi(x))\frac{h^{n+1}s(s-1)\dots(s-n)}{(n+1)!}$$

$$E_n'(x) = \frac{1}{h}\left[h^{n+1}\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\sum_{i=0}^{n}\prod_{\substack{j=0 \\ j\ne i}}^{n}(s-j) + \frac{h^{n+1}s(s-1)\dots(s-n)}{(n+1)!}\cdot\frac{d}{ds}\left(f^{(n+1)}(\xi(x))\right)\right]$$

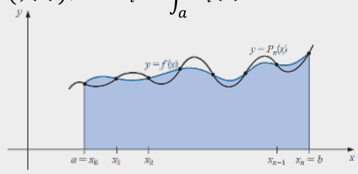
$\to E_{f'}(x) = E_n'(x) = O(h^n)$

Numerical Integral

$$\int_a^b f(x)dx = \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x)dx + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x-x_i)\, f^{(n+1)}(\xi(x))$$

$$E(f) = \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x-x_i)\, f^{(n+1)}(\xi(x)), \qquad a_i = \int_a^b L_i(x)dx$$

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + E(f)$$



Closed Newton-Cotes Formulas

n = 1: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0)+f(x_1)] - \frac{h^3}{12}f''(\xi), \qquad h = b-a$$

n = 2: Simpson's rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi), \qquad h = \frac{b-a}{2}$$

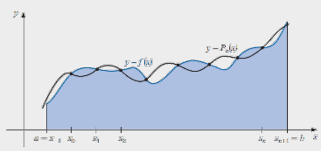
n = 3: Simpson's Three-Eighths rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)] - \frac{3h^5}{80}f^{(4)}(\xi)$$

n = 4:

$$\int_{x_0}^{x_4} f(x)dx = \frac{2h}{45}[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7(x_4)] - \frac{8h^7}{945}f^{(6)}(\xi)$$

Open Newton-Cotes Formulas



n = 0: Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi)$$

n = 1:

$$\int_{x_{-1}}^{x_2} f(x)dx = \frac{3h}{2}[f(x_0)+f(x_1)] + \frac{3h^3}{4}f''(\xi)$$

n = 2:

$$\int_{x_{-1}}^{x_3} f(x)dx = \frac{4h}{3}[2f(x_0)-f(x_1)+2f(x_2)] + \frac{14h^5}{45}f^{(4)}(\xi)$$

n = 3:

$$\int_{x_{-1}}^{x_4} f(x)dx = \frac{5h}{24}[11f(x_0)+f(x_1)+f(x_2)+11f(x_3)] + \frac{95h^5}{144}f^{(4)}(\xi)$$

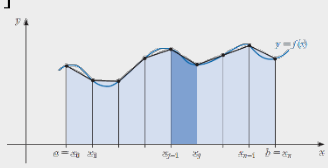
Composite Numerical Integration

Composite Trapezoidal Rule

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] + \frac{b-a}{12}h^2 f''(\mu)$$

$$T(n) = h\left[\frac{f_1+f_{n+1}}{2} + \sum_{i=2}^{n} f_i\right]$$

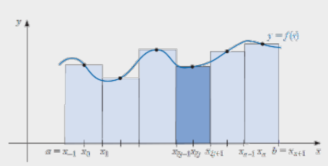
$$T(2n) = \tfrac{1}{2}[T(n)+M(n)]$$



Composite Midpoint rule

$$\int_a^b f(x)dx = 2h\sum_{j=0}^{\frac{n}{2}} f(x_{2j}) + \frac{b-a}{6}h^2 f''(\mu)$$

$$M(n) = h\sum_{i=1}^{n} f(\bar{x}_i)$$

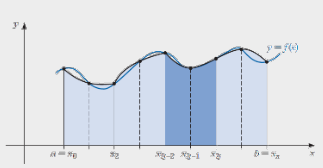


Composite Simpson's Rule

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{\frac{n}{2}-1} f(x_{2j}) + 4\sum_{j=1}^{\frac{n}{2}} f(x_{2j-1}) + f(b)\right] + \frac{b-a}{180}h^4 f^{(4)}(\mu)$$

$$S(n) = \frac{2}{3}h\sum_{i=1}^{n} f(\bar{x}_i) + \frac{h}{3}\left[\frac{f_1+f_{n+1}}{2} + \sum_{i=2}^{n} f(x_i)\right]$$

$$S(n) = \frac{2}{3}M(n) + \frac{1}{3}T(n)$$



Simpson's Rule Proof

$$\int_a^b f(x)\ dx \approx \int_a^b f(x_1)\frac{(x-x_2)\ (x-x_3)}{(x_1-x_2)\ (x_1-x_3)} + f(x_2)\frac{(x-x_1)\ (x-x_3)}{(x_2-x_1)\ (x_2-x_3)} + f(x_3)\frac{(x-x_1)\ (x-x_2)}{(x_3-x_1)\ (x_3-x_2)}\,dx$$

$$\int_a^b p(x)\ dx = hf(x_0)\int_0^2 \frac{(t-1)\ (t-2)}{(0-1)\ (0-2)}dt + hf(x_1)\int_0^2 \frac{(t-0)\ (t-2)}{(1-0)\ (1-2)}dt + hf(x_2)\int_0^2 \frac{(t-0)\ (t-1)}{(2-0)\ (2-1)}dt$$

$$\int_a^b p(x)\ dx = hf(x_0)\frac{1}{3} + hf(x_1)\frac{4}{3} + hf(x_2)\frac{1}{3}$$

Interpolating Polynomial Error Proof

Proof Note first that if $x = x_k$, for any $k = 0, 1, \ldots, n$, then $f(x_k) = P(x_k)$, and choosing $\xi(x_k)$ arbitrarily in (a, b) yields Eq. (3.3).

If $x \neq x_k$, for all $k = 0, 1, \ldots, n$, define the function g for t in $[a, b]$ by

$$g(t) = f(t) - P(t) - [f(x) - P(x)]\frac{(t-x_0)(t-x_1)\cdots(t-x_n)}{(x-x_0)(x-x_1)\cdots(x-x_n)}$$

$$= f(t) - P(t) - [f(x) - P(x)]\prod_{i=0}^{n}\frac{(t-x_i)}{(x-x_i)}.$$

Since $f \in C^{n+1}[a, b]$, and $P \in C^{\infty}[a, b]$, it follows that $g \in C^{n+1}[a, b]$. For $t = x_k$, we have

$$g(x_k) = f(x_k) - P(x_k) - [f(x) - P(x)]\prod_{i=0}^{n}\frac{(x_k-x_i)}{(x-x_i)} = 0 - [f(x) - P(x)]\cdot 0 = 0.$$

Moreover,

$$g(x) = f(x) - P(x) - [f(x) - P(x)]\prod_{i=0}^{n}\frac{(x-x_i)}{(x-x_i)} = f(x) - P(x) - [f(x) - P(x)] = 0.$$

Thus $g \in C^{n+1}[a, b]$, and g is zero at the $n+2$ distinct numbers $x, x_0, x_1, \ldots, x_n$. By Generalized Rolle's Theorem 1.10, there exists a number ξ in (a, b) for which $g^{(n+1)}(\xi) = 0$. So

$$0 = g^{(n+1)}(\xi) = f^{(n+1)}(\xi) - P^{(n+1)}(\xi) - [f(x) - P(x)]\frac{d^{n+1}}{dt^{n+1}}\left[\prod_{i=0}^{n}\frac{(t-x_i)}{(x-x_i)}\right]_{t=\xi}. \qquad (3.4)$$

However $P(x)$ is a polynomial of degree at most n, so the $(n+1)$st derivative, $P^{(n+1)}(x)$, is identically zero. Also, $\prod_{i=0}^{n}[(t-x_i)/(x-x_i)]$ is a polynomial of degree $(n+1)$, so

$$\prod_{i=0}^{n}\frac{(t-x_i)}{(x-x_i)} = \left[\frac{1}{\prod_{i=0}^{n}(x-x_i)}\right]t^{n+1} + (\text{lower-degree terms in } t),$$

and

$$\frac{d^{n+1}}{dt^{n+1}}\prod_{i=0}^{n}\frac{(t-x_i)}{(x-x_i)} = \frac{(n+1)!}{\prod_{i=0}^{n}(x-x_i)}.$$

Equation (3.4) now becomes

$$0 = f^{(n+1)}(\xi) - 0 - [f(x) - P(x)]\frac{(n+1)!}{\prod_{i=0}^{n}(x-x_i)},$$

and, upon solving for $f(x)$, we have

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{i=0}^{n}(x-x_i).$$

■ ■ ■

$f[x_0, x_1, \ldots, x_n] = f^{(n)}(\xi)/n!$ Proof

Proof Let

$$g(x) = f(x) - P_n(x).$$

Since $f(x_i) = P_n(x_i)$ for each $i = 0, 1, \ldots, n$, the function g has $n+1$ distinct zeros in $[a, b]$. Generalized Rolle's Theorem 1.10 implies that a number ξ in (a, b) exists with $g^{(n)}(\xi) = 0$, so

$$0 = f^{(n)}(\xi) - P_n^{(n)}(\xi).$$

Since $P_n(x)$ is a polynomial of degree n whose leading coefficient is $f[x_0, x_1, \ldots, x_n]$,

$$P_n^{(n)}(x) = n!\,f[x_0, x_1, \ldots, x_n],$$

for all values of x. As a consequence,

$$f[x_0, x_1, \ldots, x_n] = \frac{f^{(n)}(\xi)}{n!}.$$

■ ■ ■

Natural Spline Algorithm

To construct the cubic spline interpolant S for the function f, defined at the numbers $x_0 < x_1 < \cdots < x_n$, satisfying $S''(x_0) = S''(x_n) = 0$:

INPUT $n; x_0, x_1, \ldots, x_n; a_0 = f(x_0), a_1 = f(x_1), \ldots, a_n = f(x_n)$.

OUTPUT a_j, b_j, c_j, d_j for $j = 0, 1, \ldots, n-1$.

(Note: $S(x) = S_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$ for $x_j \le x \le x_{j+1}$.)

Step 1 For $i = 0, 1, \ldots, n-1$ set $h_i = x_{i+1} - x_i$.

Step 2 For $i = 1, 2, \ldots, n-1$ set

$$\alpha_i = \frac{3}{h_i}(a_{i+1} - a_i) - \frac{3}{h_{i-1}}(a_i - a_{i-1}).$$

Step 3 Set $l_0 = 1$; *(Steps 3, 4, 5, and part of Step 6 solve a tridiagonal linear system using a method described in Algorithm 6.7.)*
$\mu_0 = 0$;
$z_0 = 0$.

Step 4 For $i = 1, 2, \ldots, n-1$
set $l_i = 2(x_{i+1} - x_{i-1}) - h_{i-1}\mu_{i-1}$;
$\mu_i = h_i / l_i$;
$z_i = (\alpha_i - h_{i-1}z_{i-1})/l_i$.

Step 5 Set $l_n = 1$;
$z_n = 0$;
$c_n = 0$.

Step 6 For $j = n-1, n-2, \ldots, 0$
set $c_j = z_j - \mu_j c_{j+1}$;
$b_j = (a_{j+1} - a_j)/h_j - h_j(c_{j+1} + 2c_j)/3$;
$d_j = (c_{j+1} - c_j)/(3h_j)$.

Step 7 OUTPUT $(a_j, b_j, c_j, d_j$ for $j = 0, 1, \ldots, n-1)$;
STOP. ■

$$A = \begin{bmatrix} 1 & 0 & 0 & \cdots & \cdots & 0 \\ h_0 & 2(h_0+h_1) & h_1 & \ddots & & \vdots \\ 0 & h_1 & 2(h_1+h_2) & h_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & h_{n-2} & 2(h_{n-2}+h_{n-1}) & h_{n-1} \\ 0 & \cdots & \cdots & 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 0 \\ \frac{3}{h_1}(a_2 - a_1) - \frac{3}{h_0}(a_1 - a_0) \\ \vdots \\ \frac{3}{h_{n-1}}(a_n - a_{n-1}) - \frac{3}{h_{n-2}}(a_{n-1} - a_{n-2}) \\ 0 \end{bmatrix} \quad \text{and} \quad \mathbf{x} = \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix}$$

Clamped Spline Algorithm

To construct the cubic spline interpolant S for the function f defined at the numbers $x_0 < x_1 < \cdots < x_n$, satisfying $S'(x_0) = f'(x_0)$ and $S'(x_n) = f'(x_n)$:

INPUT $n; x_0, x_1, \ldots, x_n; a_0 = f(x_0), a_1 = f(x_1), \ldots, a_n = f(x_n)$; $FPO = f'(x_0)$; $FPN = f'(x_n)$.

OUTPUT a_j, b_j, c_j, d_j for $j = 0, 1, \ldots, n-1$.

(Note: $S(x) = S_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$ for $x_j \le x \le x_{j+1}$.)

Step 1 For $i = 0, 1, \ldots, n-1$ set $h_i = x_{i+1} - x_i$.

Step 2 Set $\alpha_0 = 3(a_1 - a_0)/h_0 - 3FPO$;
$\alpha_n = 3FPN - 3(a_n - a_{n-1})/h_{n-1}$.

Step 3 For $i = 1, 2, \ldots, n-1$

set $\alpha_i = \frac{3}{h_i}(a_{i+1} - a_i) - \frac{3}{h_{i-1}}(a_i - a_{i-1})$.

Step 4 Set $l_0 = 2h_0$; *(Steps 4,5,6, and part of Step 7 solve a tridiagonal linear system using a method described in Algorithm 6.7.)*
$\mu_0 = 0.5$;
$z_0 = \alpha_0 / l_0$.

Step 5 For $i = 1, 2, \ldots, n-1$
set $l_i = 2(x_{i+1} - x_{i-1}) - h_{i-1}\mu_{i-1}$;
$\mu_i = h_i / l_i$;
$z_i = (\alpha_i - h_{i-1}z_{i-1})/l_i$.

Step 6 Set $l_n = h_{n-1}(2 - \mu_{n-1})$;
$z_n = (\alpha_n - h_{n-1}z_{n-1})/l_n$;
$c_n = z_n$.

Step 7 For $j = n-1, n-2, \ldots, 0$
set $c_j = z_j - \mu_j c_{j+1}$;
$b_j = (a_{j+1} - a_j)/h_j - h_j(c_{j+1} + 2c_j)/3$;
$d_j = (c_{j+1} - c_j)/(3h_j)$.

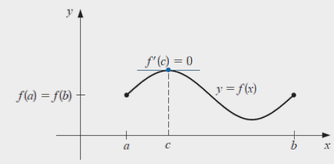
Step 8 OUTPUT $(a_j, b_j, c_j, d_j$ for $j = 0, 1, \ldots, n-1)$;
STOP. ■

$$A = \begin{bmatrix} 2h_0 & h_0 & 0 & \cdots & \cdots & 0 \\ h_0 & 2(h_0+h_1) & h_1 & \ddots & & \vdots \\ 0 & h_1 & 2(h_1+h_2) & h_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & h_{n-2} & 2(h_{n-2}+h_{n-1}) & h_{n-1} \\ 0 & \cdots & \cdots & 0 & h_{n-1} & 2h_{n-1} \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} \frac{3}{h_0}(a_1 - a_0) - 3f'(a) \\ \frac{3}{h_1}(a_2 - a_1) - \frac{3}{h_0}(a_1 - a_0) \\ \vdots \\ \frac{3}{h_{n-1}}(a_n - a_{n-1}) - \frac{3}{h_{n-2}}(a_{n-1} - a_{n-2}) \\ 3f'(b) - \frac{3}{h_{n-1}}(a_n - a_{n-1}) \end{bmatrix}, \quad \text{and} \quad \mathbf{x} = \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix}$$

Useful Theorems

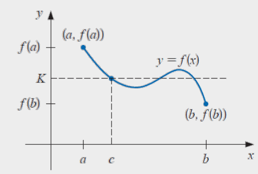
Generalized Rolle's Theorem

Suppose $f \in C[a,b]$ is n times differentiable on (a,b). If $f(x) = 0$ at the $n+1$ distinct numbers $a \le x_0 < x_1 < \ldots < x_n \le b$, then a number c in (x_0, x_n), and hence in (a,b), exists with $f^{(n)}(c) = 0$. ■



Intermediate Value Theorem

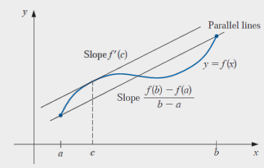
If $f \in C[a,b]$ and K is any number between $f(a)$ and $f(b)$, then there exists a number c in (a,b) for which $f(c) = K$. ■



Mean Value Theorem

If $f \in C[a,b]$ and f is differentiable on (a,b), then a number c in (a,b) exists with (See Figure 1.4.)

$$f'(c) = \frac{f(b) - f(a)}{b - a}.$$ ■



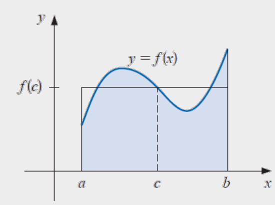
Weighted Mean Value Theorem for Integral

Suppose $f \in C[a,b]$, the Riemann integral of g exists on $[a,b]$, and $g(x)$ does not change sign on $[a,b]$. Then there exists a number c in (a,b) with

$$\int_a^b f(x)g(x)\,dx = f(c)\int_a^b g(x)\,dx.$$ ■

When $g(x) \equiv 1$, Theorem 1.13 is the usual Mean Value Theorem for Integrals. It gives the **average value** of the function f over the interval $[a,b]$ as (See Figure 1.9.)

$$f(c) = \frac{1}{b-a}\int_a^b f(x)\,dx.$$



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