### Lecture 8: Lagrange Interpolation

Solving via linear system.

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}$$

Solving via basis polynomials. Let

$$L_k(x) = \frac{(x - x_0) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)}{(x_k - x_0) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_n)} \text{ for } k = 0, 1, \dots, n. \text{ Then } P_n(x) = y_0 L_0(x) + y_1 L_1(x) + \dots + y_n L_n(x).$$

#### Error analysis.

 $\forall x \in [a, b], \exists \xi \in (\min\{x, x_0, x_1, \dots, x_n\}, \max\{x, x_0, x_1, \dots, x_n\})$ such that

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

### **Tutorial 3: Lagrange Interpolation**

**Example 1.** Construct the LIP for  $f(x) = \log_2 x$  using  $x_0 = 1/2, x_1 = 1, x_2 = 2, x_3 = 4$ . Find a bound of the absolute error for any  $x \in [1/2, +\infty)$ .

**Solution.** f(0.5) = -1, f(1) = 0, f(2) = 1, f(4) = 2. Solve using linear system to get  $a_0 = -\frac{52}{21}$ ,  $a_1 = \frac{7}{2}$ ,  $a_2 = -\frac{7}{6}$ ,  $a_3 = \frac{1}{7}$ . So  $P(x) = \frac{1}{7}x^3 - \frac{7}{6}x^2 + \frac{7}{2}x - \frac{52}{21}$ . To get an u.b for error, first find  $f^{(4)}(x) = -\frac{6}{x^4 \ln 2}$ . Note monotonicity. Hence  $|f^{(4)}(x)| \leqslant \frac{6}{(1/2)^4 \ln 2} = \frac{96}{\ln 2}$ . Thus an u.b for absolute error |P(x)-f(x)| is  $\frac{1}{4!} \times \frac{96}{\ln 2} |(x-1/2)(x-1)(x-2)(x-4)| =$  $\frac{4}{\ln 2} |(x-1/2)(x-1)(x-2)(x-4)|$ .  $\Box$ .

Result from Example 2. If nodes are equidistributed, the maximum value of  $g(x) = |(x - x_0)(x - x_1) \cdots (x - x_N)|$  must be attained in  $(x_0, x_1)$  and  $(x_{N-1}, x_N)$  (due to the symmetry).  $|g(x^*)| \leq \frac{1}{4} N! h^{N+1}$ .

#### Error estimation for equidistributed nodes.

$$|P_N(x) - f(x)| \le \frac{h^{N+1}}{4(N+1)} \max_{\xi \in [a,b]} |f^{(N+1)}(\xi)|, \text{ for all } x \in [a,b]$$

**Exercise 2.** Let  $P_n(x)$  be the LIP for  $f(x) = \cos x$  with  $x_k = kh$ ,  $k = 0, 1, \dots, n$  where  $h = \pi/(2n)$ . 1. Find a positive integer N such that  $|P_N(x) - f(x)| < 0.005$ , for all  $x \in [0, \pi/2]$ . **Solution.** For  $f(x) = \cos(x)$ ,  $\max_{\xi \in [0, \pi/2]} |f^{(N+1)}(\xi)| = 1$ . Hence it suffices to find  $\frac{h^{N+1}}{4(N+1)} < 0.005 \implies N \ge 3$ .

#### Lecture 9: Divided Differences

How to find the Lagrange polynomial.

$$\begin{split} P_n(x) &= a_0 + a_1 \left( x - x_0 \right) + a_2 \left( x - x_0 \right) \left( x - x_1 \right) + \dots + \\ a_n \left( x - x_0 \right) \left( x - x_1 \right) \cdots \left( x - x_{n-1} \right) \text{ where } a_k &= f \left[ x_0, x_1, \cdots, x_k \right] \\ \text{and } f \left[ x_0, x_1, \cdots, x_n \right] &= \frac{f \left[ x_1, x_2, \cdots, x_n \right] - f \left[ x_0, x_1, \cdots, x_{n-1} \right]}{x_n - x_0}. \\ a_0 &= f(x_0). \end{split}$$

### Lecture 10: Cubic Spline Interpolation (CSI)

How to find  $\mu_k$  and  $\lambda_k$ .

$$\mu_k = \frac{x_k - x_{k-1}}{x_{k+1} - x_{k-1}}, \quad \lambda_k = \frac{x_{k+1} - x_k}{x_{k+1} - x_{k-1}}, \quad k = 1, 2, \dots, n-1$$

Natural Boundary Conditions.  $M_0 = M_n = 0$ .

$$\begin{bmatrix} 2 & \lambda_1 \\ \mu_2 & 2 & \lambda_2 \\ & & \ddots & & \\ & \mu_3 & 2 & \ddots \\ & & & \ddots & \lambda_{n-2} \\ & & & \mu_{n-1} & 2 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ M_3 \\ \vdots \\ M_{n-2} \\ M_{n-1} \end{bmatrix} = \begin{bmatrix} 6f[x_0, x_1, x_2] \\ 6f[x_1, x_2, x_3] \\ 6f[x_2, x_3, x_4] \\ \vdots \\ 6f[x_{n-3}, x_{n-2}, x_{n-1}] \\ 6f[x_{n-2}, x_{n-1}, x_n] \end{bmatrix} = \begin{bmatrix} b^T X^T X \mathbf{b} - 2b^T X^T X \mathbf{a} + \mathbf{a}^T X^T X \mathbf{a} = (a_0, a_1, \dots, a_n)^T \\ \vdots & \vdots & \vdots \\ 1 & x_1 & x_1^2 & \dots & x_n^n \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_m & x_m^2 & \dots & x_m^n \end{bmatrix}$$
 and Clamped Boundary Conditions.

$$\mathbf{a} = (a_0, a_1, \dots, a_n)^T, \quad \mathbf{y} = (y_0, y_1, \dots, y_n)^T$$

$$2M_0 + M_1 = 6f[x_0, x_0, x_1], \quad M_{n-1} + 2M_n = 6f[x_{n-1}, x_n, x_n].$$

$$\begin{bmatrix} 2 & \lambda_0 & & & & & \\ \mu_1 & 2 & \lambda_1 & & & & \\ & \ddots & \ddots & \ddots & & \\ & & \mu_{n-1} & 2 & \lambda_{n-1} \\ & & & & \mu_n & 2 \end{bmatrix} \begin{bmatrix} M_0 \\ M_1 \\ \vdots \\ M_{n-1} \\ M_n \end{bmatrix} = \begin{bmatrix} 6f[x_0, x_0, x_1] \\ 6f[x_0, x_1, x_2] \\ \vdots \\ 6f[x_{n-2}, x_{n-1}, x_n] \\ 6f[x_{n-1}, x_n, x_n] \end{bmatrix}$$

$$\begin{split} S_k(x) &= M_{k-1} \frac{(x-x_k)^3}{6(x_{k-1}-x_k)} + M_k \frac{(x-x_{k-1})^3}{6(x_k-x_{k-1})} + A_k x + B_k. \\ A_k &= \frac{f(x_k)-f(x_{k-1})}{x_k-x_{k-1}} - \frac{1}{6} \left( M_k - M_{k-1} \right) (x_k - x_{k-1}). \\ B_k &= \frac{x_k f(x_{k-1})-x_{k-1} f(x_k)}{x_k-x_{k-1}} + \frac{1}{6} \left( M_k x_{k-1} - M_{k-1} x_k \right) (x_k - x_{k-1}). \end{split}$$

#### Piecewise Linear Interpolation (PLI). If

$$S(x) = S_k(x), \quad \text{for } x \in [x_{k-1}, x_k], k = 1, 2, \dots, n \text{ then } S_k(x) = f(x_{k-1}) \frac{x - x_k}{x_{k-1} - x_k} + f(x_k) \frac{x - x_{k-1}}{x_k - x_{k-1}}$$

Error analysis for PLI on equidistributed nodes. If  $x_k = x_0 + kh$ , then for  $x \in [x_0, x_n]$ ,

## $|f(x) - S(x)| \le \frac{1}{8} h^2 \max_{\xi \in [x_0, x_n]} |f''(\xi)|$

#### Tutorial 4: Divided Diff and CSI

Example 2: Quadratic spline interpolation. Given n+1nodes  $x_0 < x_1 < \cdots < x_{n-1} < x_n$  and a continuous function f(x). find a function S(x) such that 1. S(x) is first-order differentiable on  $(x_0, x_n)$  2. S(x) is a quadratic polynomial on  $(x_{k-1}, x_k)$  for any  $k=2,3,\cdots,n$ ; **3.** S(x) is a linear function on  $(x_0,x_1)$ . **4.**  $S(x_k) = f(x_k)$  for all  $k = 0, 1, \dots, n$ .

**Solution.** 
$$S_1(x) = f(x_0) \frac{x - x_1}{x_0 - x_1} + f(x_1) \frac{x - x_0}{x_1 - x_0}$$

$$\begin{split} & \textbf{Solution.} \ \, S_1(x) = f\left(x_0\right) \frac{x-x_1}{x_0-x_1} + f\left(x_1\right) \frac{x-x_0}{x_1-x_0}. \\ & S_k(x) = \frac{1}{2} M_k \frac{\left(x-x_{k-1}\right)^2}{x_k-x_{k-1}} + \frac{1}{2} M_{k-1} \frac{\left(x-x_k\right)^2}{x_{k-1}-x_k} + C_k, \quad k=2,3,\cdots,n. \\ & C_k = f\left(x_k\right) - \frac{1}{2} M_k \left(x_k-x_{k-1}\right). \ \, M_k = 2f\left[x_{k-1},x_k\right] - M_{k-1}. \\ & \text{Since } M_1 = S_1'\left(x_1\right) = f\left[x_0,x_1\right], \, M_k \text{ for } k=2,3,\cdots,n \text{ can be obtained iteratively.} \end{split}$$

### Lecture 11: Least Squares Approximation

**Proof of optimality.** Suppose a satisfies  $X^T X \mathbf{a} = X^T \mathbf{v}$ . Then for any vector b with the same length as a, we have  $(X\mathbf{b} - \mathbf{y})^T (X\mathbf{b} - \mathbf{y}) \geqslant (X\mathbf{a} - \mathbf{y})^T (X\mathbf{a} - \mathbf{y})$ . Proof.

$$(X\mathbf{b} - \mathbf{y})^T (X\mathbf{b} - \mathbf{y}) - (X\mathbf{a} - \mathbf{y})^T (X\mathbf{a} - \mathbf{y})$$

$$= \mathbf{b}^T X^T X \mathbf{b} - 2 \mathbf{b}^T X^T \mathbf{y} - \mathbf{a}^T X^T X \mathbf{a} + 2 \mathbf{a}^T X^T \mathbf{y}$$

$$= \mathbf{b}^T X^T X \mathbf{b} - 2 \mathbf{b}^T X^T X \mathbf{a} - \mathbf{a}^T X^T X \mathbf{a} + 2 \mathbf{a}^T X^T X \mathbf{a}$$

$$= \mathbf{b}^T X^T X \mathbf{b} - 2 \mathbf{b}^T X^T X \mathbf{a} + \mathbf{a}^T X^T X \mathbf{a} = (\mathbf{b} - \mathbf{a})^T X^T X (\mathbf{b} - \mathbf{a}) \ge 0$$

$$X = \begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_m & x_m^2 & \cdots & x_m^n \end{pmatrix} \text{ and }$$

$$\mathbf{a} = (a_0, a_1, \cdots, a_n)^T, \quad \mathbf{y} = (y_0, y_1, \cdots, y_m)^T.$$

$$X^T X a = X^T y.$$

Lecture Exercise 1. Show that the least squares approximation is unique if and only if the matrix X has full column rank, *i.e.*, the rank of X equals its number of columns. **Proof.** Note  $\operatorname{rank}(X^TX) = \operatorname{rank}(X)$ . ( $\Longrightarrow$ ) If the LSA is unique, the columns are linearly independent since we can write Xa as a unique linear combination of the columns of X. Hence the rank of the matrix is equal to the number of columns.  $(\Leftarrow)$  If Xa = b and Xa' = bthen X(a-a')=0. Since X has full rank, Xc=0 iff  $c=0 \implies a=a'$  (only the trivial solution to the homogeneous equation of linear combination of its columns exists).

Weighted LSA.  $W = \operatorname{diag} \{w_0, w_1, \cdots, w_n\}$ . Solve  $X^T W X \mathbf{a} = X^T W \mathbf{y}.$ 

### Lecture 12: Newton-Cotes Formulae (NCF)

Trapezoidal Rule.  $\int_a^b f(x) dx \approx \frac{b-a}{2} [f(a) + f(b)].$ 

Error for Trapezoidal Rule.

$$\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] - \frac{1}{12} (b-a)^{3} f''(\xi)$$

Simpson's Rule. Given f(a),  $f\left(\frac{a+b}{2}\right)$  and f(b), P(x) = $f(a) + \frac{f(b) - f(a)}{b - a}(x - a) + \left[2f\left(\frac{a + b}{2}\right) - f(b) - f(a)\right] \frac{2(x - a)(x - b)}{(b - a)^2}$ whose integral is  $\left[\frac{2}{3}f\left(\frac{a+b}{2}\right) + \frac{1}{6}f(b) + \frac{1}{6}f(a)\right](b-a)$ .

Error for Simpson's Rule

$$\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] - \frac{1}{90} \left(\frac{b-a}{2}\right)^{5} f^{(4)}(\xi)$$

Theorem 3 on Page 4. For closed Newton-Cotes formula with n+1 nodes, when n is odd and f(x) is (n+1) -th order differentiable, there exists  $\xi \in (a,b)$  such that  $\int_a^b f(x) dx =$  $\sum_{k=0}^{n} w_k f(x_k) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n s(s-1) \cdots (s-n) ds; \text{ when } n$ 

is even and 
$$f(x)$$
 is  $(n+2)$ -th order differentiable, there exists  $\xi \in (a,b)$  such that  $\int_a^b f(x) dx = \sum_{k=0}^n w_k f(x_k) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n s^2(s-1) \cdots (s-n) ds.$ 

Gaussian Elimination to find weights.

$$\begin{bmatrix} \int_a^b x^j dx = \sum_{k=0}^n w_k x_k^j, & j=0,1,\cdots,n \\ 1 & 1 & \cdots & 1 \\ x_0 & x_1 & \cdots & x_n \\ \vdots & \vdots & & \vdots \\ x_0^{n-1} & x_1^{n-1} & \cdots & x_n^{n-1} \\ x_0^n & x_1^n & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{n-1} \\ w_n \end{bmatrix} = \begin{bmatrix} \int_a^b dx \\ \int_a^b x dx \\ \vdots \\ \int_a^b x^{n-1} dx \\ c^b x^n dx \end{bmatrix}$$

How to find degree of accuracy. If  $\int_a^b x^j dx = \sum_{k=0}^n w_k x_k^j$  for  $j=0,\cdots,n$  but  $\int_a^b x^{n+1} dx \neq \sum_{k=0}^n w_k x_k^{n+1}$  then n is the degree of accuracy.

General form of NCF.  $\int_a^b f(x) dx \approx \int_a^b P(x) dx = \sum_{k=0}^n f(x_k) \int_a^b L_k(x) dx = \sum_{k=0}^n w_k f(x_k)$  where  $w_k = \int_a^b L_k(x) dx$ 

Result from Exercise 2.  $w_k = \frac{b-a}{n} \int_0^n \prod_{j=0, j \neq k}^n \frac{x-j}{k-j} dx, \quad \forall \ k = 0, \cdots, n.$ 

# Lecture 13: Composite Numerical Integration

Composite Trapezoidal Rule (CTR). Assume  $x_k - x_{k-1} = h$  for all  $k = 1, 2, \dots, n$ . Then

$$\begin{split} & \int_{a}^{b} S(x) dx = \sum_{k=1}^{n} \frac{1}{2} \left[ f\left(x_{k-1}\right) + f\left(x_{k}\right) \right] = \\ & h \left[ \frac{1}{2} f\left(x_{0}\right) + \sum_{k=1}^{n-1} f\left(x_{k}\right) + \frac{1}{2} f\left(x_{n}\right) \right] \end{split}$$

Error analysis for CTR. Suppose f(x) is second-order continuously differentiable on [a, b], and

 $\begin{array}{ll} h = \frac{b-a}{\infty}, & x_k = kh, & k = 0, 1, \cdots, n. \text{ There exists } \xi \in (a,b) \text{ such that } \\ \int_a^b f(x) \mathrm{d}x = h \left[ \frac{1}{2} f\left(x_0\right) + \sum_{k=1}^{n-1} f\left(x_k\right) + \frac{1}{2} f\left(x_n\right) \right] - \frac{b-a}{12} h^2 f''(\xi). \end{array}$ 

Composite Simpson's Rule (CSR).

$$\int_{a}^{b} f(x) dx \approx \sum_{k=1}^{n/2} \frac{h}{3} \left[ f(x_{2k-2}) + 4f(x_{2k-1}) + f(x_{2k}) \right]$$
$$= \frac{h}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2} f(x_{2k-1}) \right)$$

Error analysis for CSR. Suppose f(x) is fourth-order continuously differentiable on [a,b], and

$$h = \frac{b-a}{n}$$
,  $x_k = kh$ ,  $k = 0, 1, \cdots, n$ 

When n is an even integer, there exists  $\xi \in (a,b)$  such that  $\int_a^b f(x) dx = \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) + 4 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}) \right) - \frac{b}{3} \left( f(a) + 2 \sum_{k=1}^{n/2-1} f(x_{2k-1}$ 

$$\frac{\pi}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n} f(x_{2k}) + 4 \sum_{k=1}^{n} f(x_{2k-1}) \right)$$

$$\frac{b-a}{180} h^4 f^{(4)}(\xi)$$

Achieve abs err  $<\epsilon$ . Approximate  $\int_0^2 \sqrt{1+x^2} dx$  such that the absolute error is less than  $10^{-3}$ . For composite trapezoidal rule, b=2, a=0, abs.err  $\le \frac{1}{6}(\frac{2}{n})^2 \max_{\xi \in [0,2]} |f''(\xi)| = \frac{1}{6}(\frac{2}{n})^2$ . Hence  $n \ge 26 \implies n=26$ . For composite Simpson's rule, abs.err  $\le \frac{1}{90}(\frac{2}{n})^4 \max_{\xi \in [0,2]} |f^{(4)}(\xi)| = \frac{8}{15n^4}$ . Hence  $n \ge 4.8 \implies n=6$  because we need n to be even.

#### Tutorial 5: LSA and Integration

**Q4.** Consider the following numerical integration:  $\int_{-1}^{1} f(x) \mathrm{d}x \approx w_1 f(x_1) + w_2 f(x_2).$  How to choose  $x_1, x_2$  and  $w_1, w_2$  to achieve maximum degree of accuracy? **Solution.** For 4 unknowns, set 4 equations: set f(x) to be  $1, x, x^2, x^3$  and assume that the numerical integration is exact. Then we get equations 1.  $w_1 + w_2 = \int_{-1}^{1} 1 \mathrm{d}x = 2$ , 2.  $w_1 x_1 + w_2 x_2 = \int_{-1}^{1} x \mathrm{d}x = 0$ , 3.  $w_1 x_1^2 + w_2 x_2^2 = \int_{-1}^{1} x^2 \mathrm{d}x = \frac{2}{3}$ , 4.  $w_1 x_1^3 + w_2 x_2^3 = \int_{-1}^{1} x^3 \mathrm{d}x = 0$ . Solve to get  $w_1 = w_2 = 1, x_1 = -x_2 = \frac{1}{\sqrt{3}}$ . Degree of accuracy is found to be 3.

#### Miscellaneous

Figuring out the data points used in LSA. If the p(x) is given but the data points are incomplete, form the  $X^TXa = X^Ty$  system and select rows that look very similar to eliminate as many variables at once as possible.

The Gamma function.  $\Gamma(x) = \int_0^{+\infty} t^{x-1} e^{-t} dt$  and  $\Gamma(n) = (n-1)!$  for any positive integer n.

Linear Algebra and Calculus.

$$\frac{d}{dt} \int_{a(t)}^{b(t)} q(x) dx = q(b(t))b'(t) - q(a(t))a'(t).$$

$$\operatorname{rank}(AB) \leqslant \operatorname{rank} A = \operatorname{rank} A^T = \operatorname{rank} (A^T A)$$

**Result from T3 Eg. 2.** For  $f(x) = 1/\sqrt{x}$ ,  $f^{(N+1)}(x) = \left(-\frac{1}{2}\right)^{N+1} (2N+1)!!x^{-N-3/2}$ .

Error proofs from lectures/tutorials.

Proving Lagrange error. Define

$$g(t) = f(t) - P_n(t) - [f(x) - P_n(x)] \frac{(t-x_0)(t-x_1)\cdots(t-x_n)}{(x-x_0)(x-x_1)\cdots(x-x_n)}.$$
  $g(x_k) = 0$  so by repeated Rolle's theorem, there exists a t such that  $g^{(n+1)}(t) = f^{(n+1)}(t) - \frac{(n+1)![f(x) - P_n(x)]}{(x-x_0)(x-x_1)\cdots(x-x_n)} = 0.$  Make  $f(x) - P_n(x)$  the subject.

Proving Trapezoidal Rule error. Let  $\zeta = (a+b)/2$  and h = (b-a)/2. Define

$$g(t) = \int_{\zeta-t}^{\zeta+t} f(x) \mathrm{d}x - t[f(\zeta+t) + f(\zeta-t)], \quad r(t) = g(t) - \left(\frac{t}{h}\right)^3 g(h).$$

Idea is to approximate h with t. Then

 $g'(t) = -t \left[ f'(\zeta + t) - f'(\zeta - t) \right], \ r'(t) = g'(t) - \frac{3t^2}{\hbar^3} g(h)$  and g(0) = r(0) = r(h) = 0. Clearly r(t) is differentiable. By Rolle's theorem, we can find  $t_0 \in (0,h)$  such that  $r'(t_0) = 0$ ,

i.e.  $\frac{3t_0^2}{h^3}g(h)=g'\left(t_0\right)=-t_0\left[f'\left(\zeta+t_0\right)-f'\left(\zeta-t_0\right)\right] \text{ . By the mean value theorem, we can find } \xi\in\left(\zeta-t_0,\zeta+t_0\right) \text{ such that } f'\left(\zeta+t_0\right)-f'\left(\zeta-t_0\right)=2t_0f''(\xi). \text{ Rearrange.}$ 

Estimating the cubic spline interpolation error.

 $\max_{x \in [x_{i-1}, x_i]} |f(x) - p_3(x)| \le \frac{(h)^4}{4!} \max_{x \in [a, b]} |f^{(4)}(x)|$ . h refers to the max distance between any two points. This estimation comes from the Lagrange error.

**Tut 4 Eg. 1.** Suppose f(x) is nth order differentiable and  $x_0, x_1, \cdots, x_n$  are n+1 distinct real numbers. Show that there exists  $\xi$  between min  $\{x_0, x_1, \cdots, x_n\}$  and max  $\{x_0, x_1, \cdots, x_n\}$  such that  $f[x_0, x_1, \cdots, x_n] = \frac{f^{(n)}(\xi)}{n!}$ . **Solution.** Since the divided difference is independent of the order of its parameters, we can assume that  $x_0 < x_1 < \cdots < x_n$ . Let  $P_n(x)$  be the Lagrange interpolating polynomial of f(x) with nodes  $x_0, x_1, \cdots, x_n$ . Then  $P_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + \cdots + f[x_0, x_1, x_2, \cdots, x_n](x - x_0)(x - x_1) \cdots (x - x_{n-1})$ 

The n th derivative of  $P_n(x)$  is  $P_n^{(n)}(x) = n!f[x_0, x_1, x_2, \cdots, x_n]$ . Now we define  $g(x) = f(x) - P_n(x)$ . By the definition of interpolation, we know that  $g(x_0) = g(x_1) = \cdots = g(x_n) = 0$ . By Rolle's theorem, there exists  $\xi \in (x_0, x_n)$  such that  $g^{(n)}(\xi) = 0$ . since  $g^{(n)}(\xi) = f^{(n)}(\xi) - P_n^{(n)}(\xi) = f^{(n)}(\xi) - n!f[x_0, x_1, \cdots, x_n]$  we prove the claim by equating the above equation to zero.

**Tut 5 Eg. 1.** Show that when f is second-order differentiable on [a,b], there exists  $\xi \in (a,b)$  such that

$$\int_a^b f(x) dx - (b-a)f\left(\frac{a+b}{2}\right) = \frac{(b-a)^3}{2^4} f''(\xi).$$
 Solution. Let  $\zeta = (a+b)/2$  and define

$$g(t) = \int_{\zeta-t}^{\zeta+t} f(x) dx - 2t f(\zeta), \quad h(t) = g(t) - \left(\frac{2t}{b-a}\right)^3 g\left(\frac{b-a}{2}\right).$$
 It is obvious that  $h(0) = h\left(\frac{b-a}{2}\right) = 0$ . By Rolle's theorem, we can find  $t_0 > 0$  such that  $h'(t_0) = 0$ , i.e.,

$$g'(t_0) = 3t_0^2 \left(\frac{2}{b-a}\right)^3 g\left(\frac{b-a}{2}\right)$$
. Note that  $g'(t_0) = f(\zeta + t_0) + f(\zeta - t_0) - 2f(\zeta) = 2t_0^2 f[\zeta - t_0, \zeta, \zeta + t_0]$ . Therefore we can find  $\xi \in (\zeta - t_0, \zeta + t_0) \subset (a, b)$  such that  $f[\zeta - t_0, \zeta, \zeta + t_0] = \frac{1}{2}f''(\xi)$ . Do some substitutions.

Finding the set of x and y values for the lowest error LIP.

First find the lowest-error polynomial (LEP), which is  $p(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_m x^m$ . From Homework Q3,  $b - a \qquad b^{2-a^2} \qquad \dots \qquad b^{m+1} - a^{m+1}$ 

$$M = \begin{pmatrix} b-a & \frac{b^2 - a^2}{2} & \cdots & \frac{b^{m+1} - a^{m+1}}{m+1} \\ \frac{b^2 - a^2}{2} & \frac{b^3 - a^3}{3} & \cdots & \frac{b^{m+2} - a^{m+2}}{m+2} \\ \vdots & \vdots & \vdots \\ \frac{b^{m+1} - a^{m+1}}{m+1} & \frac{b^{m+2} - a^{m+2}}{m+2} & \cdots & \frac{b^{2m+1} - a^{2m+1}}{2m+1} \end{pmatrix} \text{ and }$$

 $\mathbf{b} = \left(\int_a^b x^0 f(x) dx, \cdots, \int_a^b x^m f(x) dx\right)^{\perp}$ . Solve Ma = b to get the coefficients of the LEP. Then reverse-engineer the Gaussian Elimination process for finding a when constructing the LIP to get x and y (possibly non-unique).

Determinant of Vandermonde matrix.

$$\det X = \prod_{i=1}^{n-1} \prod_{i=i+1}^{n} (x_j - x_i)$$