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.

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

Lecture 10: Cubic Spline Interpolation (CSI)

How to find μ_k and λ_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. $M_0 = M_n = 0$.

$$\begin{bmatrix} 2 & \lambda_1 \\ \mu_2 & 2 & \lambda_2 \\ & \mu_3 & 2 & \ddots \\ & & \ddots & \ddots & \lambda_{n-2} \\ & & & \mu_{n-1} & 2 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ M_3 \\ \vdots \\ M_{n-2} \\ M_{n-1} \end{bmatrix} = \begin{bmatrix} 6f[x_0, x_1, x_2] \\ 6f[x_1, x_2, x_3] \\ 6f[x_2, x_3, x_4] \\ \vdots \\ 6f[x_{n-3}, x_{n-2}, x_{n-1}] \\ 6f[x_{n-2}, x_{n-1}, x_n] \end{bmatrix} = \begin{bmatrix} b^T X^T X \mathbf{b} - 2\mathbf{b}^T X^T X \mathbf{a} + \mathbf{a}^T X^T X \mathbf{a} = 0 \\ \mathbf{Finding the coefficients. Let} \\ 1 & x_1 & x_1^2 & \cdots & x_n^n \\ 1 & x_1 & x_1^2 & \cdots & x_n^n \\ 1 & x_1 & x_1^2 & \cdots & x_n^n \\ 1 & x_m & x_m^2 & \cdots & x_m^n \end{bmatrix}$$
 and Clamped Boundary Conditions.

Clamped Boundary Conditions.

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

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

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

Piecewise Linear Interpolation (PLI). If

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

$$S_k(x) = f(x_{k-1}) \frac{x - x_k}{x_k - x_{k-1}} + f(x_k) \frac{x - x_{k-1}}{x_k - x_{k-1}}$$

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

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

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

$$\begin{split} &(X\mathbf{b} - \mathbf{y})^T(X\mathbf{b} - \mathbf{y}) - (X\mathbf{a} - \mathbf{y})^T(X\mathbf{a} - \mathbf{y}) \\ &= \mathbf{b}^T X^T X \mathbf{b} - 2 \mathbf{b}^T X^T \mathbf{y} - \mathbf{a}^T X^T X \mathbf{a} + 2 \mathbf{a}^T X^T \mathbf{y} \\ &= \mathbf{b}^T X^T X \mathbf{b} - 2 \mathbf{b}^T X^T X \mathbf{a} - \mathbf{a}^T X^T X \mathbf{a} + 2 \mathbf{a}^T X^T X \mathbf{a} \\ &= \mathbf{b}^T X^T X \mathbf{b} - 2 \mathbf{b}^T X^T X \mathbf{a} + \mathbf{a}^T X^T X \mathbf{a} = (\mathbf{b} - \mathbf{a})^T X^T X (\mathbf{b} - \mathbf{a}) \geqslant 0 \end{split}$$

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

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

Gaussian Elimination to find weights. TODO

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). Confusing use of h. Read carefully first

Error analysis for CTR. TODO

Composite Simpson's Rule (CSR). TODO

Error analysis for CSR. TODO

Tutorial 5: LSA and Integration

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.

Miscellaneous

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. TODO

General formulae for higher derivatives. Higher order derivatives

Error proofs from lectures/tutorials. LSA proof of optimality, the proof of errors, tutorial identities

Finding the set of x and y values for the lowest error LIP. First find the lowest-error polynomial (LEP), which is

$$p(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_m x^m. \text{ From Homework Q3},$$

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

b = $\left(\int_a^b x^0 f(x) dx, \dots, \int_a^b x^m f(x) dx\right)^2$. 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).