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

Error analysis.
$\forall x \in [a,b], \exists \xi \in (\min\{x, x_0, x_1, \cdots, x_n\}, \max\{x, x_0, x_1, \cdots, x_n\})$
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 $\frac{1}{4!} \times \frac{96}{\ln 2}|(x-1/2)(x-1)(x-2)(x-4)| = \frac{4}{\ln 2}|(x-1/2)(x-1)(x-2)(x-4)|$. $\square$.

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).
$|g(x^*)| \leqslant \frac{1}{4}N!h^{N+1}$.

Error estimation for equidistributed nodes.
$|P_N(x) - f(x)| \leqslant \frac{h^{N+1}}{4(N+1)}\max_{\xi \in [a,b]}|f^{(N+1)}(\xi)|$, for all $x \in [a,b]$

Exercise 2. Let $P_n(x)$ be the LIP for $f(x) = \cos x$ with
$x_k = kh$, $k = 0, 1, \cdots, n$ 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 $\frac{h^{N+1}}{4(N+1)} < 0.005 \implies N \geq 3$.

Lecture 9: Divided Differences

How to find the Lagrange polynomial.
$P_n(x) = a_0 + a_1(x-x_0) + a_2(x-x_0)(x-x_1) + \cdots + a_n(x-x_0)(x-x_1)\cdots(x-x_{n-1})$ where $a_k = f[x_0, x_1, \cdots, x_k]$
and $f[x_0, x_1, \cdots, x_n] = \frac{f[x_1, x_2, \cdots, x_n] - f[x_0, x_1, \cdots, x_{n-1}]}{x_n - x_0}$.
$a_0 = f(x_0)$.

Lecture 10: Cubic Spline Interpolation (CSI)

How to find μ_k and λ_k.
$\mu_k = \frac{x_k - x_{k-1}}{x_{k+1} - x_{k-1}}$, $\lambda_k = \frac{x_{k+1} - x_k}{x_{k+1} - x_{k-1}}$, $k = 1, 2, \cdots, n-1$

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

$$\begin{bmatrix} 2 & \lambda_1 & & & & \\ \mu_2 & 2 & \lambda_2 & & & \\ & \mu_3 & 2 & \ddots & & \\ & & \ddots & \ddots & \lambda_{n-2} & \\ & & & \mu_{n-1} & 2 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ M_3 \\ \vdots \\ M_{n-2} \\ M_{n-1} \end{bmatrix} = \begin{bmatrix} 6f[x_0, x_1, x_2] \\ 6f[x_1, x_2, x_3] \\ 6f[x_2, x_3, x_4] \\ \vdots \\ 6f[x_{n-3}, x_{n-2}, x_{n-1}] \\ 6f[x_{n-2}, x_{n-1}, x_n] \end{bmatrix}$$

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

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

How to find S_k.
$$S_k(x) = M_{k-1}\frac{(x-x_k)^3}{6(x_{k-1}-x_k)} + M_k\frac{(x-x_{k-1})^3}{6(x_k-x_{k-1})} + A_k x + B_k.$$
$A_k = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} - \frac{1}{6}(M_k - M_{k-1})(x_k - x_{k-1})$.
$B_k = \frac{x_k f(x_{k-1}) - x_{k-1} f(x_k)}{x_k - x_{k-1}} + \frac{1}{6}(M_k x_{k-1} - M_{k-1} x_k)(x_k - x_{k-1})$.

Piecewise Linear Interpolation (PLI). If
$S(x) = S_k(x)$, for $x \in [x_{k-1}, x_k], k = 1, 2, \cdots, n$ 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 $x \in [x_0, x_n]$,
$|f(x) - S(x)| \leq \frac{1}{8}h^2 \max_{\xi \in [x_0, x_n]}|f''(\xi)|$

Tutorial 4: Divided Diff and CSI

Example 2: Quadratic spline interpolation. Given $n+1$
nodes $x_0 < x_1 < \cdots < x_{n-1} < x_n$ 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 $k = 0, 1, \cdots, n$.
Solution. $S_1(x) = f(x_0)\frac{x-x_1}{x_0-x_1} + f(x_1)\frac{x-x_0}{x_1-x_0}$.
$S_k(x) = \frac{1}{2}M_k\frac{(x-x_{k-1})^2}{x_k-x_{k-1}} + \frac{1}{2}M_{k-1}\frac{(x-x_k)^2}{x_{k-1}-x_k} + C_k$, $k = 2, 3, \cdots, n$.
$C_k = f(x_k) - \frac{1}{2}M_k(x_k - x_{k-1})$. $M_k = 2f[x_{k-1}, x_k] - M_{k-1}$.
Since $M_1 = S_1'(x_1) = f[x_0, x_1]$, M_k for $k = 2, 3, \cdots, n$ can be
obtained iteratively.

Lecture 11: Least Squares Approximation

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

$$(Xb - y)^T(Xb - y) - (Xa - y)^T(Xa - y)$$
$$= b^T X^T X b - 2b^T X^T y - a^T X^T X a + 2a^T X^T y$$
$$= b^T X^T X b - 2b^T X^T X a - a^T X^T X a + 2a^T X^T X a$$
$$= b^T X^T X b - 2b^T X^T X a + a^T X^T X a = (b-a)^T X^T X (b-a) \geqslant 0$$

Finding the coefficients. Let
$$X = \begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_m & x_m^2 & \cdots & x_m^n \end{pmatrix} \text{ and }$$
$a = (a_0, a_1, \cdots, a_n)^T$, $y = (y_0, y_1, \cdots, y_m)^T$. Solve
$X^T X a = X^T y$.

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
$\text{rank}(X^T X) = \text{rank}(X)$. ($\implies$)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.($\impliedby$) If $Xa = b$ and $Xa' = b$
then $X(a - a') = 0$. 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. $W = \text{diag}\{w_0, w_1, \cdots, w_n\}$. Solve
$X^T W X a = X^T W y$.

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 $\int_a^b f(x)dx = \sum_{k=0}^n w_k f(x_k) + \frac{h^{n+2}f^{(n+1)}(\xi)}{(n+1)!}\int_0^n s(s-1)\cdots(s-n)ds$; 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.

$\int_a^b x^j\,dx = \sum_{k=0}^n w_k x_k^j, \quad j = 0, 1, \cdots, n$

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

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.

$\int_a^b f(x)\mathrm{d}x \approx \int_a^b P(x)\mathrm{d}x = \sum_{k=0}^n f(x_k)\int_a^b L_k(x)\mathrm{d}x = \sum_{k=0}^n w_k f(x_k)$ where $w_k = \int_a^b L_k(x)\mathrm{d}x$

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 $k = 1, 2, \cdots, n$. Then
$\int_a^b S(x)\mathrm{d}x = \sum_{k=1}^n \frac{h}{2}[f(x_{k-1}) + f(x_k)] = h\left[\frac{1}{2}f(x_0) + \sum_{k=1}^{n-1} f(x_k) + \frac{1}{2}f(x_n)\right]$

Error analysis for CTR.

Suppose $f(x)$ is second-order continuously differentiable on $[a,b]$, and $h = \frac{b-a}{\infty}, \quad x_k = kh, \quad k = 0, 1, \cdots, n$. There exists $\xi \in (a,b)$ such that
$\int_a^b f(x)\mathrm{d}x = h\left[\frac{1}{2}f(x_0) + \sum_{k=1}^{n-1} f(x_k) + \frac{1}{2}f(x_n)\right] - \frac{b-a}{12}h^2 f''(\xi).$

Composite Simpson's Rule (CSR).

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

Error analysis for CSR.

Suppose $f(x)$ is fourth-order continuously differentiable on $[a,b]$, and
$$h = \frac{b-a}{n}, \quad x_k = kh, \quad k = 0, 1, \cdots, n$$

When n is an even integer, there exists $\xi \in (a,b)$ such that
$\int_a^b f(x)\mathrm{d}x = \frac{h}{3}\left(f(a) + f(b) + 2\sum_{k=1}^{n/2-1} f(x_{2k}) + 4\sum_{k=1}^{n/2} f(x_{2k-1})\right) - \frac{b-a}{180}h^4 f^{(4)}(\xi)$

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 $\leq \frac{1}{6}(\frac{2}{n})^2 \max_{\xi \in [0,2]} |f''(\xi)| = \frac{1}{6}(\frac{2}{n})^2$. Hence $n \geq 26 \implies n = 26$. For composite Simpson's rule, abs.err $\leq \frac{1}{90}(\frac{2}{n})^4 \max_{\xi \in [0,2]} |f^{(4)}(\xi)| = \frac{8}{15n^4}$. Hence $n \geq 4.8 \implies n = 6$ 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. $w_1 + w_2 = \int_{-1}^1 1dx = 2$, 2. $w_1 x_1 + w_2 x_2 = \int_{-1}^1 xdx = 0$, 3. $w_1 x_1^2 + w_2 x_2^2 = \int_{-1}^1 x^2 dx = \frac{2}{3}$, 4. $w_1 x_1^3 + w_2 x_2^3 = \int_{-1}^1 x^3 dx = 0$. 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 $X^T X a = X^T y$ system and select rows that look very similar to eliminate as many variables at once as possible.

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

Linear Algebra and Calculus.
$\frac{d}{dt}\int_{a(t)}^{b(t)} q(x)dx = q(b(t))b'(t) - q(a(t))a'(t)$. See if I want to add LSA lemmas. . .

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. See if I want to add the lecture error proofs

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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 ξ 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
$P_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1)$
$\quad + \cdots + f[x_0, x_1, x_2, \cdots, x_n](x - x_0)(x - x_1)\cdots(x - x_{n-1})$.
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
$\int_a^b f(x)\mathrm{d}x - (b-a)f\left(\frac{a+b}{2}\right) = \frac{(b-a)^3}{24}f''(\xi)$. **Solution.** Let $\zeta = (a+b)/2$ and define
$g(t) = \int_{\zeta-t}^{\zeta+t} f(x)\mathrm{d}x - 2tf(\zeta), \quad h(t) = g(t) - \left(\frac{2t}{b-a}\right)^3 g\left(\frac{b-a}{2}\right)$. 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 $p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m$. From Homework Q3,
$$M = \begin{pmatrix} b-a & \frac{b^2-a^2}{2} & \cdots & \frac{b^{m+1}-a^{m+1}}{m+1} \\ \frac{b^2-a^2}{2} & \frac{b^3-a^3}{3} & \cdots & \frac{b^{m+2}-a^{m+2}}{m+2} \\ \vdots & \vdots & & \vdots \\ \frac{b^{m+1}-a^{m+1}}{m+1} & \frac{b^{m+2}-a^{m+2}}{m+2} & \cdots & \frac{b^{2m+1}-a^{2m+1}}{2m+1} \end{pmatrix}$$ and
$b = \left(\int_a^b x^0 f(x)dx, \cdots, \int_a^b x^m f(x)dx\right)^T$. 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).