MA 214 - Introduction to Numerical Analysis

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1 Interpolation Theory

1.1 Introduction

- Given finite set of points, reconstructing the original curve is interpolation.
- There will be obviously infinitely many curve.
- Interpolation problem Given n+1 real distinct points: x_0, x_1, \ldots, x_n and real numbers: y_0, y_1, \ldots, y_n Find a function $f : \mathbb{R} \to \mathbb{R}$ such that

$$f(x_i) = y_i$$
 for $i = 0, 1, ..., n$

Such a function is called **interpolant** and points x_i are called **interpolation points**. We attempt to rebuild original function using polynomial functions. This is called polynomial interpolation and function is polynomial interpolant.

• A polynomial is function of the form

$$p(x) = a_0 + a_1 x + \ldots + a_n x^n$$

• \mathbb{P}_n is the set of polynomials consisting of all polynomials of degree $\leq n$

1.2 Polynomial Interpolation

Theorem (Joseph-Louis Lagrange Theorem). Given n+1 data points with unique $x_i s$, then there exists a unique polynomial $p_n \in \mathbb{P}_n$ such that

$$p(x_i) = y_i$$
 for $i = 0, 1, ..., n$

Proof. (1) This can be shown by linear algebra. In a n degree polynomial, we substitute the points and get n+1 equations in n+1 variables (coeff) and all the rows are unique (since x_0, x_1, \ldots, x_n are unique), hence in AX = b, $|A| \neq 0$.

Proof. (2) Part 1: Uniqueness: If there is an interpolant, then the interpolant is unique Let there be 2 interpolants, p_n and q_n and let r(x) = p(x) - q(n),

$$r(x) = 0$$
 for $i = 0, 1, ..., n$

This contradicts the fundamental theorem of Algebra. (A polynomial of degree n can have at most n real roots). Therefore

$$r(x) = 0 \quad \forall x \in \mathbb{R}$$

 $p(x) = q(x) \quad \forall x \in \mathbb{R}$

Part 2: Existence (construction):

Given n+1 data points, build n+1 Langrange polynomials

$$L_k^n(x) = \begin{cases} 0 & \text{for } i \neq k \\ 1 & \text{for } i = k \end{cases}$$

$$L_k^n(x) = \frac{(x - x_0)...(x - x_{k-1})(x - x_{k+1})...(x - x_n)}{(x_k - x_0)...(x_k - x_{k-1})(x_k - x_{k+1})...(x_k - x_n)}$$

$$p(x) = \sum_{k=0}^n y_k L_k^n(x)$$

1.3 Closeness between functions

Given two continuous functions $f, g : [a, b] \to \mathbb{R}$, to evaluate how close the functions are consider the following

$$\max_{x \in [a,b]} |f(x) - g(x)|$$

1.4 Set of continuous Functions

C[a,b] is the set of all continuous functions on [a,b]

 ${\cal C}[a,b]$ is a infinite dimensional vector space

$$f, g \in C \Longrightarrow f + g \in C \text{ and } \lambda f \in C$$

We define norm on C[a, b] as

$$||f|| = max_{x \in [a,b]}|f(x)|$$

 $C^{k}[a,b]$ denotes the set of all functions which are continuously k-times differentiable

1.5 Polynomial Approximation and Error

Theorem (Weierstrass approximation Theorem). Given a function $f \in C[a, b]$ and given $\epsilon > 0$, there exists a polynomial p(x) such that,

$$||f(x) - p|| < \epsilon$$

Using Langrange's recipe to approximate

Take n+1 interpolation points in the [a,b] and collect the function values at all the points. We have n+1 data points. Using Lagrange polynomials, find the interpolant

Theorem (Error equation). Let $f \in C^k[a, b]$, $x_0, x_1, \ldots, x_n \in [a, b]$ and $p \in \mathbb{P}_n$ be the interpolant using these points, then for all x, there exists a $\zeta = \zeta(x) \in (a, b)$ such that

$$f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\zeta) \prod_{k=0}^{n} (x - x_k)$$

Note: Here ζ is dependent on the x, i.e, for every x you choose, ζ generally changes.

Proof. Consider the function,

$$\psi(t) = (f(t) - p(t)) \prod_{k=0}^{n} (x - x_k) - (f(x) - p(x)) \prod_{k=0}^{n} (t - x_k)$$

This n+2 roots (n+1 data points and x), applying rolle theorem's gives us that $\phi^{(1)}(t)$ has at least n+1 roots. Applying like this repeatedly on its derivatives, we get that $f^{(n+1)}$ has at least 1 root in [a,b]. Assuming the root to be ζ . We have,

$$f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\zeta) \prod_{k=0}^{n} (x - x_k)$$

Approximating the error:

Taking norm on both the sides of error equation, we have,

$$\max_{x \in [a,b]} |f(x) - p(x)| = \frac{1}{(n+1)!} ||f^{(n+1)}(\zeta) \prod_{k=0}^{n} (x - x_k)||$$
 (1)

$$\max_{x \in [a,b]} |f(x) - p(x)| \le \frac{1}{(n+1)!} ||f^{(n+1)}|| \max_{x \in [a,b]} \prod_{k=0}^{n} (x - x_k)$$
 (2)

Chebyshef interpolation points:

$$x_k = \frac{a+b}{2} + \frac{b-a}{2}cos\left(\frac{j\pi}{n}\right)$$

These points minimise $\max_{x \in [a,b]} \prod_{k=0}^{n} (x-x_k)$ and therefore prefered over equally spaced points on real line. These points can be visualised as projections of equally spaced points on the arc of the semicircle with $\frac{a+b}{2}$ as center and $\frac{(b-a)}{2}$ as radius.

1.6 Some more methods for calculating interpolant

This is similar to the linear algebra method (given as proof(1) to Joseph-Louis Lagrange Theorem) for finding the interpolant.

Consider the polynomial

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

Find the coefficients a_0, a_1, \ldots, a_n by substituting the data points. On substituting x_0 , we get a_0 , again on substituting x_1 and using a_0 , we get a_1 and so on.

• Interpolant p(x) of x_0, x_1, \ldots, x_n can be calculated using interpolants a(x) and b(x) of x_1, x_2, \ldots, x_n and $x_0, x_1, \ldots, x_{n-1}$ respectively as

$$p(x) = \frac{(x - x_0)a(x) - (x - x_n)b(x)}{x_n - x_0}$$

1.7 Divided difference - recursion relation

• Divided difference: It is the coefficient of x_n in the interpolant $p \in \mathbb{P}_n$ and denoted by $f[x_0, x_1, \dots, x_n]$.

Using Langrange polynomials, we have

$$p(x) = \sum_{k=0}^{n} f(x_k) \prod_{j=0, j \neq k}^{n} \frac{x - x_j}{x_k - x_j}$$

So the divided difference is

$$f[x_0, x_1, \dots, x_n] = \sum_{k=0}^n f(x_k) \prod_{j=0, j \neq k}^n \frac{1}{x_k - x_j}$$

Theorem (Divided difference recursion theorem).

$$f[x_0, x_1, \dots, x_{m+1}] = \frac{[f[x_1, x_2, \dots, x_{m+1}] - f[x_0, x_1, \dots, x_m]}{x_{m+1} - x_0}$$

Proof. Let p(x) be the interpolant for x_0, x_1, \ldots, x_m and q(x) be the interpolant for $x_1, x_2, \ldots, x_{m+1}$. Then,

$$L(x) = \frac{(x - x_0)q(x) + (x_{m+1} - x)p(x)}{x_{m+1} - x_0}$$

is an interpolant. Since, interpolant is unique, considering coeff of x_m we have,

$$f[x_0, x_1, \dots, x_m] = \frac{f[x_1, x_2, \dots, x_{m+1}] - f[x_0, x_1, \dots, x_m]}{x_{m+1} - x_0}$$

Theorem (Interpolant using divided differences). Suppose x_0, x_1, \ldots, x_n be the data points. Then interpolant $p \in \mathbb{P}_n$ is

$$p(x) = f[x_0] + f[x_0, x_1](x - x_0) + \dots + f[x_0, x_1, \dots, x_n] \prod_{j=0}^{n-1} (x - x_j)$$

Proof. We prove this by induction. Base case n = 0 is trivially satisfied. Assume that this is satisfied for p_k ,

$$p_k(x) = f[x_0] + f[x_0, x_1](x - x_0) + \dots + f[x_0, x_1, \dots, x_k] \prod_{j=0}^{k-1} (x - x_j)$$

Consider the polynomial $p_{k+1}(x) - p_k(x) \in \mathbb{P}_{k+1}$ which has x_0, x_1, \dots, x_k as roots. Hence,

$$p_{k+1}(x) - p_k(x) = c \prod_{j=0}^{k} (x - x_j)$$

Comparing leading coefficient on both sides, we have $c = f[x_0, x_1, \dots, x_k]$. Hence,

$$p_{k+1}(x) = f[x_0] + f[x_0, x_1](x - x_0) + \dots + f[x_0, x_1, \dots, x_{k+1}] \prod_{j=0}^{k} (x - x_j)$$

By PMI,

$$p(x) = f[x_0] + f[x_0, x_1](x - x_0) + \ldots + f[x_0, x_1, \ldots, x_n] \prod_{j=0}^{n-1} (x - x_j)$$

1.8 Weierstrass theorem consequences

• In Weierstrass approximation Theorem, take $\epsilon_n = \frac{1}{n}$. Then weierstrass theorem proves the existence of sequence of polynomials $p^{(1)}, p^{(2)}, \ldots$ such that

$$\lim_{n \to \infty} ||f - p^{(n)}|| = 0$$

• If f in not a polynomial, then

$$\lim_{n\to\infty} \text{degree of } p(n) = 0$$

1.9 Spline Interpolation

- Piece wise polynomial: $\phi \in C[a,b]$ is a piecewise polynomial function, if there exists $a = x_0 < x_1 < \ldots < x_n = b$ such that $\phi \in \mathbb{P}_m$ when $x \in [x_i, x_{i+1}]$ for all $i = 0, 1, \ldots, n$ and some m > 0.
- Piece wise polynomial ϕ need not be polynomial in whole domain.
- Splines interpolation for $f \in C[a, b]$
 - Pick some data points x_0, x_1, \ldots, x_n such that $a = x_0 < x_1 < \ldots < x_n = b$
 - Fix $m \leq n$
 - Build ϕ in each subinterval $[x_i, x_{i+1}]$ using the following conditions:

$$\phi(x_i) = f_i \quad \text{for } i = 0, 1, \dots, n$$

$$\lim_{h \to 0+} \phi(x_i - h) = \lim_{h \to 0+} \phi(x_i + h) \quad \text{for } i = 1, 2, \dots, n - 1$$

$$\lim_{h \to 0+} \frac{\mathrm{d}\phi(x_i - h)}{\mathrm{d}x} = \lim_{h \to 0+} \frac{\mathrm{d}\phi(x_i + h)}{\mathrm{d}x} \quad \text{for } i = 1, 2, \dots, n - 1$$

$$\lim_{h \to 0+} \frac{\mathrm{d}^2\phi(x_i - h)}{\mathrm{d}x^2} = \lim_{h \to 0+} \frac{\mathrm{d}^2\phi(x_i + h)}{\mathrm{d}x^2} \quad \text{for } i = 1, 2, \dots, n - 1$$

$$\vdots$$

$$\vdots$$

$$\lim_{h \to 0+} \frac{\mathrm{d}^{m-1}\phi(x_i - h)}{\mathrm{d}x^{m-1}} = \lim_{h \to 0+} \frac{\mathrm{d}^{m-1}\phi(x_i + h)}{\mathrm{d}x^{m-1}} \quad \text{for } i = 1, 2, \dots, n - 1$$

– We have (n+1)+m(n-1)=n(m+1)-(m-1) conditions. We need m-1 more conditions.

1.10 Linear Splines

Constructing linear splines:

Since the degree is only 1, we can construct the splines using the equation of straight lines between the knots (data points).

$$s_{0} = \frac{f_{1} - f_{0}}{x_{1} - x_{0}} x + \frac{x_{1}f_{0} - x_{0}f_{1}}{x_{1} - x_{0}} \qquad \text{for } x \in [x_{0}, x_{1}]$$

$$s_{1} = \frac{f_{2} - f_{1}}{x_{2} - x_{1}} x + \frac{x_{2}f_{1} - x_{1}f_{2}}{x_{2} - x_{1}} \qquad \text{for } x \in [x_{1}, x_{2}]$$

$$\vdots$$

$$s_{n-1} = \frac{f_{n} - f_{n-1}}{x_{n} - x_{n-1}} x + \frac{x_{n}f_{n-1} - x_{n-1}f_{n}}{x_{n} - x_{n-1}} \qquad \text{for } x \in [x_{n-1}, x_{n}]$$

Theorem (Linear Splines error). Let $f \in C^2[a,b]$ and $s_L(x)$ be the interpolating linear spline at (n+1) knots $a = x_0 < x_1 < \ldots < x_n = b$ and let h be the maximum subinterval length, then

$$||f - s_L|| \le \frac{h^2}{8} ||f''||$$

Proof. Consider the interval $[x_i, x_{i+1}]$, then $s_L(x)$ is the interpolating polynomial in this interval. Using the error equation for interpolating polynomials,

$$f(x) - s_L(x) = \frac{1}{2}f''(\zeta)(x - x_i)(x - x_{i+1})$$

Taking absolute value on both the sides,

$$|f(x) - s_L(x)| = \frac{1}{2} |f''(\zeta)| |(x - x_i)(x - x_{i+1})|$$

$$\leq \frac{1}{2} ||f''|| \frac{h_i^2}{4} \quad \text{where } h_i = \frac{x_{i+1} - x_i}{2}$$

$$\leq \frac{h_i^2}{8} ||f''||$$

Considering $h = max(h_i)$, then for $x \in [a, b]$

$$max_{x \in [a,b]}|f(x) - s_L(x)| \le \frac{1}{8}h^2||f''||$$

1.11 Cubic Splines

Constructing cubic splines:

$$s_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i$$

Using the conditions given in the section 1.9, we have 4n-2 equations to for 4n coefficients. We choose the other two conditions as

$$s_0''(x_0) = s_{n-1}''(x_n) = 0$$

We have 4n variables (coefficients) and 4n equations, i.e, we have a $4n \times 4n$ matrix which can be solved to get the coefficients of the spline.

We can simplify this by choosing the form of spline as

$$s_i(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i$$
 for $i = 0, 1, ..., n - 1$

We will work only with **equally spaced knots**, i.e, $x_{i+1} - x_i = const$ for i = 0, 1, ..., n - 1. We also define

$$\sigma_i = s''(x_i)$$
 for $i = 0, 1, ..., n$

After doing a lot of simplification, we get

$$\boxed{a_i = \frac{\sigma_{i+1} - \sigma_i}{6h}}$$

$$\boxed{b_i = \frac{\sigma_i}{2}}$$

$$\boxed{c_i = \frac{f_{i+1} - f_i}{h} - \frac{h}{6}(2\sigma_i + \sigma_{i+1})}$$

$$\boxed{d_i = f_i}$$

 σ_i s can be obtained by solving these equations

$$\sigma_{i-1} + 4\sigma_i + \sigma_{i+1} = \frac{6}{h^2} (f_{i-1} - 2f_i + f_{i+1})$$

This can be put in matrix form as

$$\begin{bmatrix} 4 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & 4 & 1 & \dots & 0 & 0 & 0 \\ 0 & 1 & 4 & \dots & 0 & 0 & 0 \\ \vdots & \vdots \\ 0 & 0 & 0 & \dots & 4 & 1 & 0 \\ 0 & 0 & 0 & \dots & 1 & 4 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & 4 \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \vdots \\ \sigma_{n-3} \\ \sigma_{n-2} \\ \sigma_{n-1} \end{bmatrix} = \frac{6}{h^2} \begin{bmatrix} f_0 - 2f_1 + f_2 \\ f_1 - 2f_2 + f_3 \\ f_2 - 2f_3 + f_4 \\ \vdots \\ f_{n-4} - 2f_{n-3} + f_{n-2} \\ f_{n-3} - 2f_{n-2} + f_{n-1} \\ f_{n-2} - 2f_{n-1} + f_n \end{bmatrix}$$

Theorem (Error - Cubic Splines (equispaced knots)). Let $f \in C^4[a,b]$ and $s(x) \in C^2[a,b]$ be the interpolating natural cubic spline at (n+1) equispaced knots $a = x_0 < x_1 < \ldots < x_n = b$ and let h be the subinterval length $(h = x_{i+1} - x_i)$, then

$$||f-s|| \le C||f^{(4)}||h^4$$
 for some $C > 0$

Proof. Consider the function g which is defined as $g = f - s_i$ on each subinterval $[x_i, x_{i+1}]$. Then $g(x_i) = 0$ for i = 0, 1, ..., n - 1.

We can see that the zero polynomial is the linear spline of g(x) and using the theorem Linear Splines error, we have

$$||g - 0|| \le \frac{h^2}{8} ||g''||$$

 $||f - s|| \le \frac{h^2}{8} ||f'' - s''||$

Assuming that $||f'' - s''|| \le Ch^2 ||f^{(4)}||$, we have

$$||f - s|| \le Ch^4 ||f^{(4)}||$$
 for some $C > 0$

2 Numerical Integration

2.1 Introduction

• Given f be a real valued function, we want to evaluate

$$\int_{a}^{b} f(x)dx$$

• If we can find its antiderivative F(x), then we can use the fundamental theorem of calculus and evaluate it. But finding antiderivate is not so straightforward.

$$\int_{a}^{b} f(x)dx = F(b) - F(a)$$

2.2 Newton-Cotes Formula

Let $f(x): [a,b] \to \mathbb{R}$ and $p(x) \in \mathbb{P}_n$ be the polynomial interpolant using the data points $a = x_1 < x_2 < \ldots < x_n = b$, then the definite integral $\int_a^b f(x)dx$ can be approximated as

$$\int_{a}^{b} f(x)dx \approx \int_{a}^{b} p(x)dx$$

$$= \int_{a}^{b} \sum_{i=0}^{n} f(x_{i})L_{i}(x)dx$$

$$= \sum_{i=0}^{n} f(x_{i}) \int_{a}^{b} L_{i}(x)dx$$

Let $x_i = a + ih$ for i = 0, 1, ..., n and x = a + th for $t \in [0, n]$, then we have,

$$\int_{a}^{b} L_{i}(x)dx = \int_{a}^{b} \prod_{k=0, k \neq i}^{n} \frac{x - x_{k}}{x_{i} - x_{k}} dx = \int_{0}^{n} \prod_{k=0, k \neq i}^{n} \frac{t - k}{i - k} h dt = h \int_{0}^{n} \varphi_{i}(t) dt = h w_{i}$$

where
$$w_i = \int_0^n \varphi_i(t)dt$$
 and $\varphi_i(t) = \prod_{k=0}^n \sum_{k\neq i}^n \frac{t-k}{i-k}$

Then,

$$\boxed{\int_a^b f(x)dx \approx h \sum_{i=0}^n w_i f(x_i)}$$

Note: w_i s are independent of f, end points a and b and h. w_i s are dependent on only dependent on n. **Note**: w_i s are symmetric i.e,

$$w_k = w_{n-k}$$

Trapezium rule (n = 1):

$$\int_{a}^{b} f(x)dx \approx \frac{b-a}{2}(f(a)+f(b))$$

Simpson's rule (n = 2):

$$\int_{a}^{b} f(x) dx \approx \frac{h}{3} \left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right)$$

2.3 Newton-Cones formula error

We use the Error equation, for interpolation polynomial to calculate the error in Newton-Cotes formula.

$$|I_f - I_P| = \left| \int_a^b f(x) - p(x) dx \right|$$

$$\leq \int_a^b |f(x) - p(x)| dx$$

$$|I_f - I_P| \le \frac{1}{(n+1)!} ||f^{(n+1)}|| \int_a^b \prod_{i=0}^n |x - x_i| dx$$

For trapezium rule (n=1)

$$|I_f - I_{P_1}| \le \frac{1}{2} ||f''|| \int_a^b |(x - a)(x - b)| dx$$

= $\frac{1}{12} ||f''|| (b - a)^3$

For simpson's rule (n=2)

$$|I_f - I_{P_2}| \le \frac{1}{6}||f'''|| \int_a^b |(x-a)(x-\frac{a+b}{2})(x-b)| dx$$
$$= \frac{1}{192}||f''||(b-a)^4$$

(//todo: stricter bound for siemsons rule)

2.4 Convergence of the approximation

- The difference $|I_f I_{P_n}|$ does not converge to 0 as we increase n. This is (crudely) because the weights sometimes takes negative values.
- A similar approximation which converges as n increases is Gaussian quadratures.

$$G_n(f) = \sum_{i=0}^{n} W_i f(x_i)$$

where weights W_i are

$$W_{i} = \int_{a}^{b} (L_{i}(x))^{2} dx = \int_{a}^{b} \left[\prod_{k=0, k \neq i}^{n} \frac{x - x_{k}}{x_{i} - x_{k}} \right]^{2} dx$$

Here, the points x_k s are **not** equally spaces. x_k s are the roots of Legendre Polynomials

2.5 Composites Rule

Similar to the splines case, we approximate the integral using Newton-Cotes formula in each subinterval.

• Composite Trapezoidal Rule: We divide the interval [a, b] into m subintervals and apply trapezoidal rule in each subinterval.

$$\int_{a}^{b} f(x)dx \approx \int_{a}^{b} C_{p_{1}}dx$$

$$= h(\frac{1}{2}f(a) + \frac{1}{2}f(a+h)) + h(\frac{1}{2}f(a+h) + \frac{1}{2}f(a+2h)) + \dots + h(\frac{1}{2}f(a+(m-1)h) + \frac{1}{2}f(b))$$

$$= h(\frac{1}{2}f(a) + f(a+h) + f(a+2h) + \dots + f(a+(m-1)h) + \frac{1}{2}f(b))$$

• Composite Simpson's Rule: We divide the interval [a, b] into 2m subintervals and apply simpons' rule.

$$\int_{a}^{b} f(x)dx \approx \int_{a}^{b} C_{p_{2}}dx$$

$$= h(\frac{1}{3}f(a) + \frac{4}{3}f(a+h) + \frac{1}{3}f(a+2h)) + h(\frac{1}{3}f(a+2h) + \frac{4}{3}f(a+3h) + \frac{1}{3}f(a+4h))$$

$$+ \dots + h(\frac{1}{3}f(a+(2m-2)h) + \frac{4}{3}f(a+(2m-1)h) + \frac{1}{3}f(b))$$

$$= h(\frac{1}{3}f(a) + \frac{4}{3}f(a+h) + \frac{2}{3}f(a+2h) + \frac{4}{3}f(a+3h) + \frac{2}{3}f(a+4h) + \dots$$

$$+ \frac{2}{3}f(a+(2m-2)h) + \frac{4}{3}f(a+(2m-1)h) + \frac{1}{3}f(b))$$

2.6 Error - Composites Rule

- To get an estimate of the error $|I_f C_{p_n}|$, we sum the error in each subinterval.
- For composite trapezoid rule,

$$|I_f - C_{p_1}| \le \sum_{i=0}^m \frac{1}{12} ||f''|| h^3$$

= $\frac{1}{12} ||f''|| h^2 (b-a)$

3 Ordinary Differential Equation