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

  $$f(x_i) = y_i \qquad \text{for } i = 0, 1, \ldots, n$$

  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_is, then there exists a unique polynomial $p_n \in \mathbb{P}_n$ such that*

$$p(x_i) = y_i \qquad \textit{for } i = 0, 1, \ldots, n$$

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 $r(x) = p(x) - q(n)$,

$$r(x) = 0 \text{ for } i = 0, 1, \ldots, n$$

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]
$C[a, b]$ is a infinite dimensional vector space

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

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*

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

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,

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

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

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
  $$p(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \ldots + a_n(x - x_0)...(x - x_{n-1})$$
  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 $f[x_0, x_1 \ldots, x_n]$.
  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
  $$f[x_0, x_1, \ldots, x_n] = \sum_{k=0}^{n} f(x_k) \prod_{j=0, j\neq k}^{n} \frac{1}{x_k - x_j}$$

Theorem (Divided difference recursion theorem)**.**

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

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,

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

□

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*

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

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

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

Consider the polynomial $p_{k+1}(x) - p_k(x) \in \mathbb{P}_{k+1}$ which has $x_0, x_1, \ldots, x_k$ 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 $c = f[x_0, x_1, \ldots, x_k]$. Hence,

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

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 Time complexity of the algorithms

- Langrange's method - $O(n^2)$: Computing each Langrange polynomial can be done in $O(n)$ (Finding the coefficients given roots can be done in $O(nlog^2(n))$). We need to do to this n times. So, $O(n^2)$.
- Divided differences - $O(n^2)$: Summing operations in each stage - $n+(n-1)+(n-2)+\ldots+1$. Hence, $O(n^2)$.
- Divided difference can be considered better because we can extend from n to n+1 and so on without discarding previous computation.

1.9 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

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

1.10 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:

$$\begin{aligned}
\phi(x_i) &= f_i && \text{for } i = 0, 1, \ldots, n \\
\lim_{h\to 0+} \phi(x_i - h) &= \lim_{h\to 0+} \phi(x_i + h) && \text{for } i = 1, 2, \ldots, n-1 \\
\lim_{h\to 0+} \frac{\mathrm{d}\phi(x_i - h)}{\mathrm{d}x} &= \lim_{h\to 0+} \frac{\mathrm{d}\phi(x_i + h)}{\mathrm{d}x} && \text{for } i = 1, 2, \ldots, n-1 \\
\lim_{h\to 0+} \frac{\mathrm{d}^2\phi(x_i - h)}{\mathrm{d}x^2} &= \lim_{h\to 0+} \frac{\mathrm{d}^2\phi(x_i + h)}{\mathrm{d}x^2} && \text{for } i = 1, 2, \ldots, n-1 \\
&\vdots \\
\lim_{h\to 0+} \frac{\mathrm{d}^{m-1}\phi(x_i - h)}{\mathrm{d}x^{m-1}} &= \lim_{h\to 0+} \frac{\mathrm{d}^{m-1}\phi(x_i + h)}{\mathrm{d}x^{m-1}} && \text{for } i = 1, 2, \ldots, n-1
\end{aligned}$$

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

1.11 Linear Splines

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

$$\begin{aligned}
s_0 &= \frac{f_1 - f_0}{x_1 - x_0}x + \frac{x_1 f_0 - x_0 f_1}{x_1 - x_0} && \text{for } x \in [x_0, x_1] \\
s_1 &= \frac{f_2 - f_1}{x_2 - x_1}x + \frac{x_2 f_1 - x_1 f_2}{x_2 - x_1} && \text{for } x \in [x_1, x_2] \\
&\vdots \\
s_{n-1} &= \frac{f_n - f_{n-1}}{x_n - x_{n-1}}x + \frac{x_n f_{n-1} - x_{n-1} f_n}{x_n - x_{n-1}} && \text{for } x \in [x_{n-1}, x_n]
\end{aligned}$$

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*

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

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,

$$\begin{aligned} |f(x) - s_L(x)| &= \frac{1}{2}|f''(\zeta)||(x - x_i)(x - x_{i+1})| \\ &\leq \frac{1}{2}||f''||\frac{h_i^2}{4} \qquad \text{where } h_i = \frac{x_{i+1} - x_i}{2} \\ &\leq \frac{h_i^2}{8}||f''|| \end{aligned}$$

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

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

□

1.12 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 1.10, 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

$$s_i(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i \qquad \text{for } i = 0, 1, \ldots, n-1$$

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

$$\sigma_i = s''(x_i) \qquad \text{for } i = 0, 1, \ldots, n$$

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

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

This can be put in matrix form as

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

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*

$$\boxed{||f - s|| \leq C||f^{(4)}||h^4 \qquad \textit{for some } C > 0}$$

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 $i = 0, 1, \ldots, n-1$.
We can see that the zero polynomial is the linear spline of $g(x)$ and using the theorem Linear Splines error, we have

$$\begin{aligned} ||g - 0|| &\leq \frac{h^2}{8}||g''|| \\ ||f - s|| &\leq \frac{h^2}{8}||f'' - s''|| \end{aligned}$$

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

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

□

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

$$\begin{aligned}
\int_a^b f(x)dx &\approx \int_a^b p(x)dx \\
&= \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x)dx \\
&= \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)dx
\end{aligned}$$

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

$$\int_a^b L_i(x)dx = \int_a^b \prod_{k=0,k\neq i}^{n} \frac{x - x_k}{x_i - x_k}dx = \int_a^b \prod_{k=0,k\neq i}^{n} \frac{t-k}{i-k}hdt = h\int_a^b \varphi_i(t)dt = hw_i$$

$$\text{where } w_i = \int_a^b \varphi_i(t)dt \text{ and } \varphi_i(t) = \prod_{k=0,k\neq i}^{n} \frac{t-k}{i-k}$$

Then,

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

Trapezium rule ($n = 1$):

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

Simpson's rule ($n = 2$):

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