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

[a, b] is a immitte 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

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

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

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

$$d_i = f_i$$

 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)

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

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

3.1 Uniqueness and Existence Theorem

Theorem (Cauchy-Lipschitz-Picard). Consider the initial value problem

$$y' = f(t, y) \qquad y(t_0) = y_0$$

- 1. If the function f is continuous for $t_0 \le t \le T$ and $y_0 C \le y \le y_0 + C$ for some constants T, C > 0.
- 2. If the function f satisfies lipschitz condition.

Lipschitz condition: There exists a constant L > 0 such that

$$|f(t,u) - f(t,v)| \le L|u - v|$$

for all $t \in [t_0, T]$ and $u, v \in [y_0 - C, y_0 + C]$

Then there exists a unique solution $y(t) \in C^1[t_0,T]$ such that

$$y' = f(t, y) \qquad y(t_0) = y_0$$

Lipschitz condition imposes the condition that the slope of the function f (with t treated as constant) is bounded.

3.2 Integral Formula

Consider the initial value problem

$$y' = f(t, y) \qquad y(t_0) = y_0$$

Interating with y from y_0 to y and t from t_0 to t

$$y = y_0 + \int_{t_0}^{t} f(s, y(s)) ds$$

3.3 Order of Numerical Method

Consider a numerical method given by the recurrence relation

$$y_{i+1} = F(t, f, y_0, y_1, \dots, y_i, y_{i+1})$$

Order of the numerical method is said to be p if

$$y(t_{i+1}) - F(t, f, y(t_0), y(t_1), \dots, y(t_i), y(t_{i+1})) = O(h^{p+1})$$

This in some sense represents order of error that is included while approximating from y_i to y_{i+1} since we use exact values while computing y_{i+1} and get the difference between $y(t_{i+1})$ and t_{i+1} . Order can also be interpreted as the highest degree of polynomial which is exactly recovered after approximating the solution using the numerical method. (Here, order is the degree of the polynomial and not function f)

3.4 Global error

In an interval [0,T] for a given h>0, there are $\left\lceil \frac{T}{h}\right\rceil+1$ are equally spaced mesh points. Let

$$e_{n,h} = y_{n,h} - y(t_n)$$

3.5 Convergence of Numerical Method

A numerical method is said to be convergent if

$$\lim_{h \to 0^{+}} \max_{i=0,1,\dots,\left[\frac{T}{h}\right]} |e_{i,h}| = 0$$

3.6 Euler Method

To approximate the solution, we divide the interval [0,T] into n mesh points, i.e, $t_i = ih$, where $h = \frac{T}{n}$. At the mesh point t_i , we find approximations y_i for exact solution $y(t_i) = y(t_{i-1}) + \int_{t_{i-1}}^{t_i} f(s, y(s)) ds$ using

$$y_i = y_{i-1} + hf(t_{i-1}, y_{i-1})$$
 for $i = 1, 2, ..., n$

Order:

$$y(t_{i+1}) - F(t, f, y(t_0), y(t_1), \dots, y(t_n), y(t_{n+1}))$$

$$= y(t_{i+1}) - (y(t_i) + hf(t_i, y(t_i)))$$

$$= y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(\zeta) - (y(t_i) + hf(t_i, y(t_i)))$$
 using taylor's expansion
$$= \frac{y''(\zeta)}{2}h^2$$

$$= O(h^2)$$

Hence, the order of Euler's method is 1.

Using the above result and lipschitz condition, we can prove that

$$|e_{i,h}| \le \frac{Ch}{\lambda}((1+\lambda h)^i - 1)$$
 for $i = 0, 1, \dots, [\frac{T}{h}]$

Since, $|e_{i,h}| = O(h)$, so $\lim_{h\to} |e_{i,h}| = 0$ and hence euler's method is convergent. Since the global error converges to zero at the rate of h^1 , the order of convergence of Euler method is said to be 1.

3.7 Trapezoidal Rule

The recurrence relation for trapezoidal rule is implicit.

$$y_i = y_{i-1} + \frac{h}{2}(f(t_{i-1}, y_{i-1}) + f(t_i, y_i))$$

Order:

$$y(t_{i+1}) - F(t, f, y(t_0), y(t_1), \dots, y(t_n), y(t_{n+1}))$$

$$= y(t_{i+1}) - (y(t_i) + \frac{h}{2}(y'(t_i) + y'(t_{i+1})))$$

$$= y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(t_i) + \frac{h^3}{6}y'''(\zeta_1) - (y(t_i) + \frac{h}{2}(y'(t_i) + y'(t_i) + hy''(t_i) + \frac{h^2}{2}y'''(\zeta_2)))$$

$$= (\frac{y'''(\zeta_1)}{6} - \frac{y'''(\zeta_2)}{4})h^3$$

$$= O(h^3)$$

Hence, the order of Trapezoidal Rule is 2.

Using the above result and lipschitz condition, we can prove that

$$|e_{i,h}| \le \frac{Ch^2}{\lambda} \left(\left(\frac{1 + \frac{\lambda h}{2}}{1 - \frac{\lambda h}{2}} \right)^i - 1 \right) \quad \text{for i } = 0, 1, \dots, \left[\frac{T}{h} \right]$$

Since, $|e_{i,h}| = O(h^2)$, so $\lim_{h\to} |e_{i,h}| = 0$ and hence trapezoidal method is convergent. Since the global error converges to zero at the rate of h^2 , the order of convergence of trapezoidal method is said to be 2.

3.8 Multistep Methods

• Simpson's Rule We have

$$y(t_{i+1}) - y(t_{i-1}) = \int_{t_{i-1}}^{t_{i+1}} f(t, y) dt$$

We use the simpsons rule to approximate the integral

$$y_{t_{i+1}} = y_{t_{i-1}} + \frac{h}{3} \left(f(t_{i-1}, y_{i-1} + 4f(t_i, y_i) + f(t_{i+1}, y_{i+1}) \right)$$

Note: Here, $h = t_{i+2} - t_i$

• Adam Bashfort Method: (Explicit 4 step method)

$$y_{i+4} = y_{i+3} + \frac{h}{24} (55f(t_{i+3}, y_{i+3}) - 59f(t_{i+2}, y_{i+2} + 37f(t_{i+1}, y_{i+1} - 9f(t_i, y_i))))$$

• Adam Moulton Method: (Implicit 3 step method)

$$y_{i+3} = y_{i+2} + \frac{h}{24} (9f(t_{i+3}, y_{i+3}) + 19f(t_{i+2}, y_{i+2} - 5f(t_{i+1}, y_{i+1} - 9f(t_i, y_i))))$$

3.9 General multistep method

Any s step method is of the form

$$\sum_{m=0}^{s} a_m y_{i+m} = h \sum_{m=0}^{s} b_m f(t_{i+m}, y_{i+m}) \quad \text{for i} = 0, 1, 2, \dots$$

Here, a_m, b_m, s are constants (independent of h,i and f) For any s step method we need s starting points $(y_0, y_1, y_2, \dots, y_{s-1})$

3.10 Constructing s step method

Adams method of constructing s step method:

- 1. Take the s points $t_i, t_{i+1}, \ldots, t_{i+s-1}$ and corresponding values (approximated by using y_i instead of $y(t_i)$) $f(t_i, y_i), f(t_{i+1}, y_{i+1}), \ldots, f(t_{i+s-1}, y_{i+s-1})$ and find the interpolating polynomial
- 2. Integrate the obtained polynomial between t_{i+s-1} to t_{i+s} for obtaining $y_{i+s} y_{i+s-1}$, i.e.

$$y_{i+s} - y_{i+s-1} = \int_{t_{i+s-1}}^{t_{i+s}} \sum_{m=0}^{s-1} f(t_{i+m}, y_{i+m}) \prod_{p=0, p \neq m}^{s-1} \left(\frac{t - t_{i+p}}{t_{i+m} - t_{i+p}} \right) dt$$

On simplifying we have

$$y_{i+s} - y_{i+s-1} = h \sum_{m=0}^{s-1} b_m f(t_{i+m}, y_{i+m})$$

where
$$b_m = \int_{s-1}^{s} \prod_{p=0, p \neq m}^{s-1} \left(\frac{x-p}{m-p} \right) dx$$

3.11 Order of s step method

Theorem. The order of s step method is p if

1.

$$\sum_{m=0}^{s} a_m = 0$$

2.

$$\sum_{m=0}^{s} a_m m^k = k \sum_{m=0}^{s} b_m m^{k-1} \qquad \text{for } k = 1, 2, \dots, p$$

3.

$$\sum_{m=0}^{s} a_m m^{p+1} \neq (p+1) \sum_{m=0}^{s} b_m m^p$$

So to compute order, we keep on checking if $\sum_{m=0}^{s} a_m m^k = k \sum_{m=0}^{s} b_m m^{k-1}$ while increasing, if this condition is not satisfied for k (first time), then k-1 is the required order.

3.12 Convergence

Consider the general s step method

$$\sum_{m=0}^{s} a_m y_{i+m} = h \sum_{m=0}^{s} b_m f(t_{i+m}, y_{i+m}) \quad \text{for i} = 0, 1, 2, \dots$$

The associated characteristics polynomials are

$$\rho(z) = \sum_{m=0}^{s} a_m z^m \qquad \qquad \sigma(z) = \sum_{m=0}^{s} b_m z^m$$

Theorem (Dahlquist equivalence theorem). A s-step method is convergent iff

- 1. The method is of order $p \geq 0$
- 2. The roots of the characteristic polynomial $\rho(z)$ lies in the closed unit disc in the complex plane, with any roots that lie on the unit circle being simple.

3.13 Range-Kutta Method

To compute y_{n+1} using y_n we approximate the integral $\int_{t_n}^{t_{n+1}}$. From the interval $[t_n, t_{n+1}]$, we take some data points $t_n + c_1 h$, $t_n + c_2 h$, ..., $t_n + c_n h$ (note that the last point may not be equal to t_{n+1}) and compute the value using quadrature weights (similar to the case when we used a 2 data points in trapezoidal rule, 3 in simpsons rule etc).

$$y_{n+1} = y_n + \sum_{i=1}^{\nu} b_i f(c_i h, \zeta_i) \qquad \zeta_i \approx y(c_i, h)$$

Here, we compute the ζ_{ν} using the data points in the interval before $t_n + c_i h$, i.e, we use the points $t_n + c_1 h, t_n + c_2 h, \ldots, t_n + c_{\nu-1} h$ to compute ζ_{ν}

$$\zeta_{\nu} = y_n + h \sum_{i=0}^{\nu-1} a_{\nu,i} f(t_n + c_i h, \zeta_i)$$

To control the order of the of a numerical method

- 1. We will compute $y_{n+1} y_n$ and $y(t_{n+1}) y(t_n)$.
- 2. We will assume that the error is zero upto the nth step, i.e, $y_n = y(t_n)$, then the difference of the above two terms is the error in the (n+1)th step
- 3. For the order to be p, we should adjust the all the terms of order p and less than p to zero, so that $y_{n+1} y(n+1) = O(h^{p+1})$

4 Numerical Solutions to system of Linear Equations

4.1 Gauss Elimination

(I skipped some details)

- 1. We transform the given matrix (augumented matrix) into row echelon form using elementary row transformations, i.e, we eliminate the variable x_i from all the equations below it by multiplying with appropriate factor and subtracting.
- 2. Solve the system by back substitution, i.e, start from the last row variable and work your way up.

 $x_i = \frac{b_i - \sum_{j=i+1}^n a_{ij}}{a_{ii}}$

Factorisation Methods

Instead of solving Ax = B, we factorise A = BC, then solve for $y \in R^n$ in By = b and then $x \in R^n$ in Cx = y. The trick is that B and C should be "simple" matrices, so that we can simplify our problem.

4.2 LU Factorisation

Lower and Upper triangular matrices

- If a lower triangular matrix is invertible, then the inverse is also a lower triangular matrix with diagonal entries being reciprocals of the original diagonal entries. Same goes with upper triangular matrices
- The product of two lower triangular matrices is also a lower triangular matrix. Same goes with upper triangular.

We factorise A into

$$A = LU$$

L is lower triangular matrix with diagonal entries equal to 1 and U is upper-triangular matrix.

- This is same as Gauss elimination method.
- \bullet We obtain the L matrix and U matrix from the process.
- L matrix is the matrix of multipliers, i.e, the numbers we multiply the above rows to get rid of the rows below. m_{ij} is the number we multiply the above row to get rid of jth variable in the ith column.

Theorem. Let A be a matrix such that all of its diagonal submatrices are invertible. Then there exists a unique pair of matrices L and U with L being lower-triangular with diagonal entries equal to unity and U being upper-triangular such that

$$A = LU$$

4.3 Chelosky Factorisation

Positive Definite:

Let A be a real, symmetric matrix, then the following conditions are equivalent:

- 1. A is positive definite
- 2. $\langle Ay, y \rangle \ge 0$ for all $y \in \mathbb{R}^n$
- 3. All the eigen values of A are positive.
- 4. All the pivots are positive
- 5. The determinates of all the diagonal submatrices are positive

Ref: Positive definite matrices

Theorem. Let A be a real, symmetric and positive definite matrix, then there exists a unique lower triangular matrix B with positive diagonal entries such that

$$A = BB^T$$

B is called the Chelosky factor

Practical approach: Take matrix B in terms of variables b_{ij} and multiply with B^T . Compare the terms to find the unknowns (prefably left to right).

4.4 QR Factorisation

In this we factor as

$$A = QR$$

where Q is a orthogonal matrix $(Q^T = Q)$ and R is a upper triangular matrix

Theorem. Every invertible matrix can be factorised as A = QR

Ref: Some theory and example

5 Norms

5.1 Norms on \mathbb{R}^n

• l^p norm for $p \in [1, \infty]$

$$||x||_{l^p} = (\sum_{i=1}^n |x_i|^p)^{\frac{1}{p}}$$

• l^{∞} norm

$$||x||_{l^{\infty}} = \max_{1 \le i \le n} |x_i|$$

• Two norms ||.|| and ||.||' are said to be equivalent if there exist positive constants such that

$$C'||x|| \le ||x||' \le C||x||$$
 for all $x \in R^n$

• All norms are equivalent on \mathbb{R}^n

$$||x||_{l^{\infty}} \le ||x||_{l^{p}} \le n^{\frac{1}{p}} ||x||_{l^{\infty}}$$

$$||x||_{l^2} \le ||x||_{l^1} \le \sqrt{n}||x||_{l^2}$$

5.2 Norms on matrix $M_{m \times n}$

• Treating matrix as a mn vector,

$$||A||_{l^p} = \left(\sum_{i=1}^m \sum_{j=1}^n |A_{ij}|^p\right)^{\frac{1}{p}}$$

$$||A||_{l^{\infty}} = \max_{1 \leq i \leq m, 1 \leq j \leq n} |A_{ij}|$$

• norm can be defined as $(l^p \text{ norm on each column and } l^q \text{ norm on the resultant vector})$

$$||A||_{L_{p,q}} = \left(\sum_{j=1}^{n} \left(\sum_{i=1}^{m} |A_{ij}|^{p}\right)^{\frac{q}{p}}\right)^{\frac{1}{q}}$$

• Taking p = 2, we get **frobenius norm**

$$||A||_{l^2} = \left(\sum_{j=1}^n \sum_{i=1}^m |A_{ij}|^2\right)^{\frac{1}{2}}$$

• Matrix Norm: A norm ||.|| is said to be matrix norm if

$$||AB|| \le ||A||||B||$$
 for all $A, B \in M_n(R)$

Frobenius norm is a matrix norm

$$||AB||_{l^2} < ||A||_{l^2} ||B||_{l^2}$$

• Subordinate Matrix Norm: Let A be a M_n matrix, then

$$||A||_p = \sup_{x \in \mathbb{R}^n - \{0\}} \frac{||Ax||_{l^p}}{||x||_{l^p}} = \sup_{y \in \mathbb{R}^n, ||y|| = 1} ||Ay||_{l^p}$$

• Subordinate Matrix norm is a matrix norm

• Subordinate matrix norm of identity matrix is always 1

$$||I_n|| = \sup_{x \in \mathbb{R}^n - \{0\}} \frac{||I_n x||}{||x||} = 1$$

- Frobenius norm is a matrix norm but not a subordinate matrix norm (since frobenius norm of identity matrix is not 1)
- Subordinate matrix norm (p=2) of unitary matrix $(A^T=A^{-1})$ is 1

$$||A||_2 = 1$$
 if A is a unitary matrix

• $||.||_2$ norm is invariant is invariant under multiplication by unitary matrices $(A^T = A^{-1})$

$$||AB||_2 = ||BA||_2 = ||B||_2$$

• For a diagonal matrix $A = diag(a_1, a_2, \dots, a_n)$

$$||A||_2 = \max_{1 \le i \le n} |a_i|$$

5.3 Normal Matrices

A matrix $A \in M(C)$ is called a normal matrix

$$AA^* = A^*A$$

where A^* is the adjoint of A

Theorem. A matrix $A \in M(C)$ is a normal matrix iff it can be expressed as

$$A = Udiag(\lambda_1, \lambda_2, \dots, \lambda_n)U^*$$

where $\lambda_1, \lambda_2, \dots, \lambda_n$ are eigenvalues of A and U is a unitary matrix

• For a normal matrix $A \in M_n(C)$

$$||A||_2 = ||Udiag(\lambda_1, \lambda_2, \dots, \lambda_n)U^*||_2 = \max_{1 \le i \le n} |\lambda_i|$$

5.4 Spectral Radius

The maximum of the eigen values of a matrix A is calle the spectral radius

$$\rho(A) = \max_{1 \le i \le n} |\lambda_i|$$

- For a normal matrix A, $||A||_2 = \rho(A)$
- For any **matrix norm** ||.|| on M(C), we have

$$\rho(A) \le ||A||$$

• Note: The above inequality may not hold for non matrix norm

Theorem. For any matrix $A \in M_n$ and for any $\epsilon > 0$, there exists a subordinate matrixnorm ||.|| such that

$$||A|| \le \rho(A) + \epsilon$$

This matrix norm depends on A and ϵ

5.5 Hermitian Matrix

• A matrix is said to be hermitian if

$$A = A^*$$

• A matrix is hermitian iff there exist unitary matrix U and real eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, such that

$$A = Udiag(\lambda_1, \lambda_2, \dots, \lambda_n)U^*$$

- For any matrix A, AA^* is a hermitian matrix and also its eigenvalues are always positive.
- Singular Values: The singular values of a matrix are the square roots of eigenvalues of AA*.
- For a normal matrix, singular values are the modulli of its eigenvalues.

5.6 Subordinate matrix norm computation

• Subordinate matrix norm $||.||_1$ (also called column sum)

$$||A||_1 = \max_{1 \le j \le n} (\sum_{i=0}^n |A_{ij}|)$$

i.e, ||.|| is same as the maximum column sum (absolute values)

• Subordinate matrix norm $||.||_{\infty}$

$$||A||_{\infty} = \max_{1 \le i \le n} (\sum_{j=0}^{n} |A_{ij}|)$$

i.e, ||.|| is same as the maximum row sum (absolute values)

• For any matrix $A \in M_n(C)$, subordinate $||A||_2$ norm is

 $||A||_2 = \text{largest singular value of A}$

6 Matrix Sequences

6.1 Convergence

A sequence A_k is said to converge to a limit A if

$$\lim_{k \to \infty} ||A^{(k)} - A|| = 0$$

The choice of norm is irrelevant as all norms are equivalent

Theorem. The following are equivalent

- 1. $\lim_{k\to\infty} A^k = 0$
- 2. $\lim_{k\to\infty} A^k x = 0$
- 3. The spectral radius of $\rho(A) \leq 1$
- 4. there exists at least one subordinate matrix such that $||A|| \leq 1$

Theorem. 1. The geometric series $\sum_{k=0}^{\infty} A^k$ converges iff the $\rho(A) < 1$

2. If the geometric series converges, then

$$\sum_{k=0}^{\infty} A^k = (I - A)^{-1}$$

Miscellaneous note: If all the eigen values are non zero, then the matrix is invertible

Theorem.

For any matrix B in the neighbourhood of A, i.e,

$$||A - B|| < \frac{1}{||A^{-1}||}$$

then B is invertible

6.2 Relative Error

For a vector $y \in \mathbb{C}^n$ and $\tilde{y} \in \mathbb{C}^n$ its pertubed value, relative is error is defined as

Relative Error
$$=\frac{||y-\tilde{y}||}{||y||}$$

6.3 Condition Number

For a invertible matrix A, condition number is defined as

$$cond(A) = ||A||||A^{-1}||$$

- $cond(A) \ge 1$
- $cond(A) = cond(A^{-1})$
- $cond(\alpha A) = cond(A)$ for all $\alpha \neq 0$
- Condition number acts as a amplifying factor Let $A_{\epsilon}=A+\epsilon B$ for some B and $\epsilon<<1$, $b_{\epsilon}=b+\epsilon c$ for some $c\in C^n$

$$\frac{||x_{\epsilon} - x||}{||x||} \leq ||A||||A^{-1}|| \left(\frac{||b_{\epsilon} - b||}{||b||} + \frac{||A_{\epsilon} - A||}{||A||} \right) + O(\epsilon^{2})$$

- A matrix is said to be well conditioned if $cond(A) \approx 1$ and ill conditioned if cond(A) >> 1
- Consider a matrix A with μ_{max} and μ_{min} be its maximum and minimum singular value, then

$$cond_2(A) = \frac{\mu_{max}}{\mu_{min}}$$