Numerical Mathematics 1 Lecture Notes (2024/2025)

Griffin Reimerink

Contents

---

1 Approximating functions

1.1 Polynomial interpolation

Theorem *Taylor's theorem*

Let $y(x)$ be a function and $T_n y(x)$ its degree n Taylor approximation at x_0:

$$T_n y(x) = \sum_{n=0}^{\infty} \frac{y^{(n)}(x_0)}{n!}(x - x_0)^n = y(x_0) + y'(x_0)(x - x_0) + \frac{y''(x_0)}{2}(x - x_0)^2 + \dots$$

Then the error is equal to:

$$y(x) - T_n y(x) = y^{(n+1)}(\xi)\frac{(x - x_0)^{n+1}}{(n+1)!}$$

for some ξ between x and x_0.

Algorithm *Lagrange interpolation*

If the value of $y(x)$ at points $x_0, x_1, \dots \in [a, b]$ is known, then we can approximate $y(x)$ by a **Lagrange interpolator** (denoted $\Pi_n y$) by solving the following system of equations:

$$\begin{bmatrix} y(x_0) \\ y(x_1) \\ \vdots \\ y(x_n) \end{bmatrix} = \begin{bmatrix} 1 & x_0 & \dots & x_0^n \\ 1 & x_1 & \dots & x_1^n \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & \dots & x_n^n \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{bmatrix}$$

The matrix is called the **Vandermonde matrix**.

Degree 1 Lagrange interpolation

$$\Pi_1 y(x) = y(x_0)\frac{x - x_1}{x_0 - x_1} + y(x_1)\frac{x - x_0}{x_1 - x_0}$$

Proposition

$$\Pi_n y(x) = \sum_{k=0}^{n} \varphi_k(x) y(x_k) \qquad \varphi_k(x) = \prod_{\substack{j=0 \\ j \neq k}} \frac{x - x_j}{x_k - x_j}$$

The functions φ_k are called the **Lagrange basis functions**.

Proposition

The Lagrange interpolator Π_n is unique and the Vandermonde matrix is invertible.

Proposition *Lagrange interpolation error*

There exists $\xi \in (a, b)$ (which depends on x and n) such that:

$$y(x) - \Pi_n y(x) = \frac{y^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i) \qquad \forall x \in [a, b]$$

For this error formula, the function needs to be continuously differentiable $n + 1$ times.
This is not necessary for the computation of Π_n.

1.2 Numerical integration

Proposition

The following equations are equivalent:

$$\dot{y} = f(y(t), t),\ y(t_0) = y_0 \iff y(t) = y_0 + \int_{t_0}^{t} f(y(s), s)\,\mathrm{d}s$$

Definition

$$I(f) := \int_a^b f(x)\,\mathrm{d}x \qquad \mathbb{P}_d := \{\text{polynomials of degree } d\}$$

Approximation of an integral

We can approximate the integral $I(f)$ by integrating the Lagrange interpolant of f:

$$\tilde{I} = \int_a^b \tilde{f}(x)\,\mathrm{d}x = \sum_{i=0}^{m} f(x_i) \int_a^b \varphi_i(x)\,\mathrm{d}x$$

Definition

$\tilde{I}(f)$ has **degree of exactness** d if

$$\tilde{I}(f) = I(f) \text{ for } f \in \mathbb{P}_d \quad \text{and} \quad \text{there exists } q \in \mathbb{P}_{d+1} \text{ such that } I(q) \neq \tilde{I}(q)$$

Theorem

The integral computed using a degree n polynomial interpolation has degree of exactness $n \leq d \leq 2(n+1)$

1.2.1 Newton-Cotes quadratures

Definition *Newton polynomial*

$$w_n = \prod_{i=1}^{n} (x - x_i)$$

Newton-Cotes quadratures

$$\tilde{I}(f) = \sum_{i=0}^{n} w_i f(a + h_i) \qquad h_i = x_{i+1} - x_i$$

$n = 0$: **midpoint rule**

$$\tilde{I}(f) = f\left(\frac{a+b}{2}\right)(b-a) \qquad d = 1$$

$n = 1$: **trapezoidal rule**

$$\tilde{I}(f) = \frac{f(a) + f(b)}{2}(b-a) \qquad d = 1$$

$n = 2$: **Simpson's rule**

$$\tilde{I}(f) = \frac{b-a}{6} f(a) + \frac{2}{3}(b-a) f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} f(b) \qquad d = 3$$

Theorem

For Newton-Cotes quadratures with even n, we have $d \geq n+1$

Theorem *Mean value theorem for integrals*

Let f, g be continuous on $[a, b]$, and g does not change sign. Then there exists $\xi \in (a, b)$ such that

$$\int_a^b f(x) g(x)\,\mathrm{d}x = f(\xi) \int_a^b g(x)\,\mathrm{d}x$$

1.2.2 Gauss-Legendre quadrature

Definition *Inner product of functions on* $[-1,1]$

$$\langle f,g\rangle = \int_{-1}^{1} f(x)g(x)\,\mathrm{d}x$$

Definition *Legendre polynomials*

$$\begin{aligned}
L_0(x) &= 1\\
L_1(x) &= x - \frac{\langle x, L_0\rangle}{\langle L_0, L_0\rangle}L_0(x) = x\\
L_2(x) &= x^2 - \frac{\langle x^2, L_0\rangle}{\langle L_0, L_0\rangle}L_0(x) - \frac{\langle x^2, L_1\rangle}{\langle L_1, L_1\rangle}L_1(x) = x^2 - \frac{1}{3}\\
&\vdots\\
L_n(x) &= x^n - \sum_{j=0}^{n-1}\frac{\langle x^n, L_j\rangle}{\langle L_j, L_j\rangle}L_j(x)
\end{aligned}$$

Proposition *Properties of the Legendre polynomials*

1. The Legendre polynomials are orthogonal to each other.
2. The degree n Legendre polynomial is orthogonal to x^k for $k < n$.
3. $\langle x^n, L_n\rangle = \langle L_n, L_n\rangle$
4. $\mathbb{P} = \operatorname{span}\{L_0, L_1, \ldots, L_n\}$

Proposition

L_n is orthogonal to any polynomial of degree $n-1$.

Theorem

For $n > 0$, the roots of L_n all have multiplicity 1, and they are located in $[-1,1]$.

Theorem *Euclid's division lemma for polynomials*

Given two univariate polynomials p and $h \neq 0$, there exist two unique polynomials q (the quotient) and r (the remainder) which satisfy:

$$p(x) = q(x)h(x) + r(x) \qquad \deg(q) + \deg(h) = \deg(p) \qquad \deg(r) < \deg(h)$$

Definition *Gauss-Legendre quadrature*

$$\tilde{I}_m^G(f) = \sum_{k=1}^{m}\omega_k f(x_k)$$

where $x_1, \ldots, x_n$ are the roots of L_n, and $\omega_1, \ldots, \omega_n$ the weights that allow to integrate exactly polynomials of degree $m-1$ computed with the linear system:

$$\begin{bmatrix} \int_{-1}^{1} 1\,\mathrm{d}x \\ \int_{-1}^{1} x\,\mathrm{d}x \\ \vdots \\ \int_{-1}^{1} x^{m-1}\,\mathrm{d}x \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_m \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{m-1} & x_2^{m-1} & \cdots & x_m^{m-1} \end{bmatrix} \begin{bmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_m \end{bmatrix}$$

The degree of exactness of the Gauss-Legendre quadrature with m nodes is $d = 2m-1$.
Since it is built on a degree $n = m-1$ polynomial interpolation, the degree of exactness is equal to $2n+1$.

2 Root-finding

2.1 Fixed-point iterations

Definition *Fixed point*

Let ϕ_f be a function dependent on f. We call x^* a **fixed point** of ϕ_f if $\phi_f(x^*) = x^*$.

Requirements of ϕ_f for root-finding

To use fixed points of ϕ_f to find roots of f, we need the following conditions:

- ϕ_f has at least 1 fixed point.
- f has a root at a fixed point of ϕ_f
- All terms of ϕ_f have the same dimension

The general form of a function that satisfies these conditions is:

$$\phi_f(x) = x + g(f(x)) \qquad g(0) = 0$$

Proposition *Existence of fixed points*

If the following conditions hold, ϕ_f has at least 1 fixed point.

1. ϕ_f maps $[a, b]$ to $[a, b]$.
2. ϕ_f is continuous on $[a, b]$.

Note: these conditions do not imply uniqueness of the fixed point.

Definition *Lipschitz continuity*

ϕ is **Lipschitz-continuous** within $[a, b]$ if there exists $L > 0$ such that

$$|\phi(x) - \phi(y)| \leq L|x - y| \qquad \text{for all } x, y \in [a, b]$$

Proposition

$$\phi \text{ is } C^1 \implies \phi \text{ is Lipschitz} \implies \phi \text{ is } C^0$$

Definition *Contraction*

ϕ is a **contraction** if it is Lipschitz with $L < 1$

Theorem *Uniqueness of fixed points*

Let ϕ_f be a function satisfying the following conditions:

1. ϕ_f maps $[a, b]$ to $[a, b]$.
2. ϕ_f is a contraction on $[a, b]$.

Then ϕ_f has a <u>unique</u> fixed point on $[a, b]$.

Theorem

Let ϕ be a contraction that maps $[a, b]$ to $[a, b]$. Define $x^{(k+1)} = \phi(x_k)$ for some initial guess x_0.
Then $x^{(k)}$ converges to the unique fixed point x^* of ϕ as $k \to \infty$.

Definition *Newton method*

Let $f \in C^2$ and $f'(x) \neq 0$ on $[a, b]$. Then we can define the following function and iteration method:

$$\phi_N := x - \frac{f(x)}{f'(x)} \qquad x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

2.2 Convergence speed

Definition *Convergence rate and factor*

$x^{(k)}$ is **convergent** to x^* with **convergence rate** p and **convergence factor** $C^{(k)}$ if

$$|x^{(k+1)} - x^{(k)}| \leq C^{(k)}|x^{(k)} - x^*|^p$$

Proposition *Convergence speed*

If ϕ' is continuous and $\phi'(x^*) \neq 0$, we have $p = 1$ and the following asymptotic convergence factor:

$$C^{(\infty)} = |\phi'(x^*)|$$

If ϕ'' is continuous and $\phi'(x^*) = 0$, we have $p = 2$ and the following asymptotic convergence factor:

$$C^{(\infty)} = \frac{|\phi''(x^*)|}{2}$$

If $\phi^{(0)}, \dots, \phi^{(p)}$ are continuous and $\phi^{(m)}(x^*) = 0$ for all $1 \leq m < p$, then the convergence order is p and the asymptotic convergence factor is

$$C^{(\infty)} = \frac{|\phi^{(p)}(x^*)|}{p!}$$

Proposition *Convergence speed of the Newton method*

For the Newton method, if $f'(x^*) \neq 0$, then we have $p \geq 2$.

2.3 Systems of equations

Solving systems of equations using the Newton method

We can solve the linear system $F(x) = 0$ (with F, x and 0 vector-valued) with the following iteration method:

$$x^{(k+1)} = x^{(k)} - J_F^{-1}(x^{(k)})F(x^{(k)})$$

where J_F denotes the Jacobian matrix.

3 Solutions of ODEs

Cauchy problem

Let $I \subset \mathbb{R}$ and $f : I \times \mathbb{R}^n \to \mathbb{R}^m$. Find $y : I \to \mathbb{R}^n$ such that:

$$\begin{cases} y'(t) = f(t, y(t)) & t \in I \\ y(t_0) = y_0 & t_0 \in I \end{cases}$$

This can be written as:

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

Numerically, our goal is to find values y_k such that $y_k \approx y(t_k)$ for some values of $t_k \in I$.
To do this, we iteratively solve the following equation:

$$y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f(s, y(s))\,\mathrm{d}s$$

The Cauchy problem has a unique solution if f is continuous with respect to t and Lipschitz with respect to y.

3.1 The β-method

Forward Euler method (explicit method)

$$u_0 = y_0 \qquad u_{n+1} = u_n + f(t_n, u_n) \cdot (t_{n+1} - t_n)$$

Backward Euler method (implicit method)

$$u_0 = y_0 \qquad u_{n+1} = u_n + f(t_{n+1}, u_{n+1}) \cdot (t_{n+1} - t_n)$$

Midpoint method (implicit method)

$$u_0 = y_0 \qquad u_{n+1} = u_n + f\left(\frac{t_n + t_{n+1}}{2}, \frac{u_n + u_{n+1}}{2}\right) \cdot (t_{n+1} - t_n)$$

β-method

Let h be the length of each interval $[t_n, t_{n+1}]$.

$$u_0 = y_0 \qquad u_{n+1} = u_n + hf(t_{n+\beta}, (1-\beta)u_n + \beta u_{n+1})$$

This method is explicit for $\beta = 0$ and implicit for $\beta > 0$.

3.2 Asymptotic stability

Definition *Asymptotic stability*

Let h be the length of each interval t_n, t_{n+1}. A method is:

- **unconditionally stable** if $u_n \xrightarrow{n\to\infty} 0$ for all $h > 0$
- **conditionally stable** if $u_n \xrightarrow{n\to\infty} 0$ for all $0 < h < h_{\text{crit}}$

Stability of the β-method (linear case)

For $f(t, y) = \lambda y$, the β-method is conditionally stable for $0 < \beta < \frac{1}{2}$ and unconditionally stable for $\frac{1}{2} \le \beta \le 1$.

In the case $0 < \beta < \frac{1}{2}$, we have stability if $h < \dfrac{\mathrm{Re}(\lambda)}{(\beta - \frac{1}{2})|\lambda|^2}$

3.3 Error analysis

Error causes

There are three steps that can possibly cause an error:

$$y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f(s, y(s))\,\mathrm{d}s$$

$\Downarrow$ (1) Integral approximation

$$y_{n+1} = y_n + hf(t_{n+\beta}, y(t_{n+\beta}))$$

$\Downarrow$ (2) Approximate $y(t_{n+\beta})$ by a linear combination

$$y_{n+1} = y_n + hf(t_{n+\beta}, (1-\beta)y_n + \beta y_{n+1})$$

$\Downarrow$ (3) Replace y_n by its approximation u_n

$$u_{n+1} = u_n + hf(t_{n+\beta}, (1-\beta)u_n + \beta u_{n+1})$$

Truncation error

For step (1), we have the following errors, called **truncation errors**:

$$\beta = 0 \quad \tau_n = \frac{y''(\xi)}{2}h^2 \qquad \beta = \frac{1}{2} \quad \tau_n \leq \frac{y'''(\xi)}{24}h^3 + \frac{5}{8}h^3 L_f \max_\alpha |y''(\alpha)| \qquad \beta = 1 \quad \tau_n = \frac{-y''(\xi)}{2}h^2$$

L_f is the Lipschitz constant of f with respect to y.
The order of the truncation errors is:

$$\tau_n = \begin{cases} \mathcal{O}(h^2) & \beta \in \{0, 1\} \\ \mathcal{O}(h^3) & \beta = \frac{1}{2} \end{cases}$$

Amplification factor

Let $f(t, y) = \lambda y$. Then we can write the β-method as

$$u_{n+1} = A_\beta(\lambda h)u_n + \frac{hg(t_{n+\beta})}{1 - \beta h\lambda} \qquad A_\beta(z) = \frac{1 + (1 - \beta)z}{1 - \beta z}$$

A_β is called the **amplification factor**. We have asymptotic stability if $|A_\beta| < 1$.

Error of the β-method in the linear case

If $f(t, y) = \lambda y$, then we have the following error:

$$\begin{aligned} |y_{n+1} - u_{n+1}| &\leq |y_{n+1} - \hat{u}_{n+1}| + |\hat{u}_{n+1} - u_{n+1}| \\ &\leq \frac{\tau_h(h)}{1 - \lambda\beta h} + A_\beta(h\lambda)|y_n - u_n| \end{aligned}$$

By computing the recursion, we get the following explicit bound for the error:

$$|y_{n+1} - u_{n+1}| \leq \frac{\max_n\{\tau_n(h)\}}{|1 - \beta h\lambda|} \cdot \frac{1 - |A_\beta|^{n+1}}{1 - |A_\beta|}$$

For a fixed time T, we have

$$e(T) \leq \frac{\tau(h)}{-\lambda h}(1 - e^{\lambda T}) = \begin{cases} \mathcal{O}(h) & \beta \in \{0, 1\} \\ \mathcal{O}(h^2) & \beta = \frac{1}{2} \end{cases}$$

3.4 Systems of ODEs

System of ODEs

$$\begin{aligned} y_1' &= f_1(t, y_1(t), y_2(t) \ldots, y_n(t)) \qquad y_1(t_0) = y_{1,0} \\ y_2' &= f_2(t, y_1(t), y_2(t) \ldots, y_n(t)) \qquad y_1(t_0) = y_{2,0} \\ &\vdots \\ y_N' &= f_N(t, y_1(t), y_2(t) \ldots, y_n(t)) \qquad y_1(t_0) = y_{N,0} \end{aligned}$$

β-method for systems

$$\vec{U}_{n+1} = \vec{U}_n + h\vec{F}(t_{n+\beta}, (1 - \beta)\vec{U}_n + \beta\vec{U}_{n+1}) \qquad \vec{U}_n = \begin{bmatrix} u_{1,n} \\ u_{2,n} \\ \vdots \\ u_{N,n} \end{bmatrix} \qquad \vec{F} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}$$

For $\beta = 0$, the β-method is explicit and can be applied in the same way as before.
For other values of β, we can apply the Newton method on the following function:

$$\vec{R}(\vec{U}_{n+1}) = \vec{U}_{n+1} - \vec{U}_n - h\vec{F}(t_{n+\beta}, (1 - \beta)\vec{U}_n + \beta\vec{U}_{n+1}) = 0$$

For the initial guess we use $\vec{U}_n$. If the Newton method does not converge, we can decrease h until it converges.

Jacobian of R

$$J_R(X) = I - h\beta J_f(X)$$

3.5 Asymptotic stability for linear systems

Matrix amplification factor

Consider the linear system $\vec{y}' = A\vec{y}$. We can write the β-method as:

$$\vec{U}_{n+1} = \underbrace{(I - hA\beta)^{-1}(I + h(1-\beta)A)}_{G}\vec{U}_n$$

We have asymptotic stability if $\|G\| < 1$.

Asymptotic stability for linear systems

Consider the linear system $\vec{y}' = A\vec{y}$.
For $\beta < 1/2$, we have asymptotic stability if

$$h < \frac{\mathrm{Re}(\lambda_i)}{(\beta - \frac{1}{2})|\lambda_i|^2} \qquad \text{for all eigenvalues } \lambda_i \text{ of } A$$

3.6 Asymptotic stability for nonlinear ODEs

Direct Lyapunov method

If there exists a function $\mathbb{R}^n \to \mathbb{R}$ such that

- $V(y) = 0$ if and only if $y = 0$
- $V(y) > 0$ if and only if $y \neq 0$
- $\frac{\mathrm{d}}{\mathrm{d}t}V(y(t)) < 0$ for all $y \neq 0$

then $\lim\limits_{t\to\infty} y(t) = 0$.

Index