Chapter 3
Numerical Differentiation and Integration

Songting Luo

Department of Mathematics
Iowa State University

MATH 561 Numerical Analysis

Numerical Integration; Basics

Definition ((Weighted) Numerical Quadrature)

Let $t_1, \dots, t_n$ be n distinct points in $[a, b]$ and $w_1, \dots, w_n \in \mathbf{R}$. We call

$$\int_a^b f(t)w(t)dt \approx \sum_{k=1}^{n} w_k f(t_k) \tag{1}$$

a (weighted) numerical quadrature with $t_1, \dots, t_n$ quadrature points and $w_1, \dots, w_n$ coefficients.
The quadrature (1) is exact for f if $\int_a^b f(t)w(t)dt = \sum_{k=1}^{n} w_k f(t_k)$.

Definition (Degree of Accuracy (Exactness, Precision))

The degree of accuracy (exactness, precision) of a quadrature formula (1) is the largest positive integer d s.t. the formula is exact for x^k, for each $k = 0, 1, \dots, d$.

Interpolatory Quadrature

Definition (Interpolatory Quadrature)

The interpolatory quadrature associated with $n+1$ distinct points $t_0, t_1, \ldots, t_n$ in $[a, b]$ is the numerical quadrature

$$\int_a^b f(t)w(t)dt \approx \sum_{k=0}^{n} w_k f(t_k) \tag{2}$$

with

$$w_k = \int_a^b l_k(t)w(t)dt, \quad k = 0, 1 \ldots, n,$$

where $l_0, \ldots, l_n$ are the Lagrange basis polynomials associated with $t_0, \ldots, t_n$.

The Newton-Cotes Formulas; Error Formula

Theorem (Error Formula for Closed Newton-Cotes Formula)

Consider a closed Newton-Cotes Formula with nodes $t_0, \ldots, t_n$, $h = (b-a)/n$:

- *If n is even and $f \in C^{n+2}[a,b]$, there exists $\xi \in (a,b)$ s.t.,*

$$\int_a^b f(t)dt - \sum_{k=0}^{n} w_k f(t_k) = \frac{f^{(n+2)}(\xi)}{(n+2)!}\mu_n,$$

  where $\mu_n = \int_a^b t(t-t_0)\cdots(t-t_n)dt = h^{n+3}\int_0^n t^2(t-1)\cdots(t-n)dt$.

- *If n is odd and $f \in C^{n+1}[a,b]$, there exists $\eta \in (a,b)$ s.t.*

$$\int_a^b f(t)dt - \sum_{k=0}^{n} w_k f(t_k) = \frac{f^{(n+1)}(\eta)}{(n+1)!}\nu_n,$$

  where $\nu_n = \int_a^b (t-t_0)\cdots(t-t_n)dt = h^{n+2}\int_0^n t(t-1)\cdots(t-n)dt$.

The Newton-Cotes Formulas; Error Formula

Theorem (Error Formula for Open Newton-Cotes Formula)

Consider a open Newton-Cotes Formula with nodes $t_0, \ldots, t_n$, $h = (b-a)/(n+2)$:

- *If* n *is even and* $f \in C^{n+2}[a,b]$, *there exists* $\xi \in (a,b)$ *s.t.,*

$$\int_a^b f(t)dt - \sum_{k=0}^{n} w_k f(t_k) = \frac{f^{(n+2)}(\xi)}{(n+2)!}\mu_n,$$

  where $\mu_n = h^{n+3}\int_{-1}^{n+1} t^2(t-1)\cdots(t-n)dt$.

- *If* n *is odd and* $f \in C^{n+1}[a,b]$, *there exists* $\eta \in (a,b)$ *s.t.*

$$\int_a^b f(t)dt - \sum_{k=0}^{n} w_k f(t_k) = \frac{f^{(n+1)}(\eta)}{(n+1)!}\nu_n,$$

  where $\nu_n = h^{n+2}\int_{-1}^{n+1} t(t-1)\cdots(t-n)dt$.

Peano Kernel and Error Representation

Theorem

Assume the degree of exactness of a numerical quadrature

$$\int_a^b f(t)dt \approx \sum_{k=0}^{n} w_k f(t_k)$$

is m. *Then*

$$\int_a^b f(t)dt - \sum_{k=0}^{n} w_k f(t_k) = \int_a^b \tilde{K}_m(s) f^{(m+1)}(s)ds, \quad \forall f \in C^{m+1}[a,b],$$

where

$$\tilde{K}_m(s) = \frac{1}{m!}[\int_a^b (t-s)_+^m dt - \sum_{k=0}^{n} w_k (t_k - s)_+^m].$$

(Terms in the square brackets are error of approximating integral of $(t-s)_+^m$ with the quadrature formula)

Can We Do Better?

Definition ((Weighted) Numerical Quadrature)

Let $t_1, \ldots, t_n$ be n distinct points in $[a, b]$ and $w_1, \ldots, w_n \in \mathbf{R}$. We call

$$\int_a^b f(t)w(t)dt \approx \sum_{k=1}^{n} w_k f(t_k) \tag{3}$$

a (weighted) numerical quadrature with $t_1, \ldots, t_n$ quadrature points and $w_1, \ldots, w_n$ coefficients.

Remark: For $(n+1)$-point Newton-Cotes formula, the degree of exactness is $n+1$ if n is even, and n if n is odd.

Question: for the quadrature formula (3), can we choose the n nodes and n weights to have degree of exactness as high as possible? Since there are $2n$ parameters, we may expect to have degree of exactness as high as $2n-1$?

An Example

Find t_1, t_2 and w_1, w_2 such that the quadrature

$$\int_{-1}^{1} f(t)dt \approx w_1 f(t_1) + w_2 f(t_2)$$

has degree of exactness 3. Using Method of Undetermined Coefficients.
Set up 4 equations for the 4 unknowns
Degree of exactness 3 implies the quadrature is exact for $1, t, t^2, t^3$.
Solution: $w_1 = 1, w_2 = 1$, $t_1 = -\frac{\sqrt{3}}{3}, t_2 = \frac{\sqrt{3}}{3}$, i.e.,

$$\int_{-1}^{1} f(t)dt \approx f(-\frac{\sqrt{3}}{3}) + f(\frac{\sqrt{3}}{3})$$

(Weighted) Gaussian Quadrature; Gauss Formulae

Theorem

Given an integer k with $0 \leqslant k \leqslant n$, the quadrature formula (3) *has degree of exactness $d = n - 1 + k$ if and only if the following conditions are satisfied:*

- *The formula* (3) *is interpolatory*
- *The node polynomial $\omega_n(t) \equiv \prod_{k=1}^{n}(t - t_k)$ satisfies $\int_a^b \omega_n(t)p(t)w(t)dt = 0$ for all $p \in \mathbf{P}_{k-1}$.*

The second condition implies ω_n is orthogonal to $\mathbf{P}_{k-1}$.
Clearly, $k \leqslant n$, which implies maximum degree of exactness $d_{\max} = 2n - 1$.
A good guess is ω_n is the n-th orthogonal polynomial $\pi_n(t; w)$; then $t_1, \ldots, t_n$ are zeros of $\pi_n(t; w)$. This optimal formula is called the Gaussian quadrature formula associated with the weight function w.

(Weighted) Gaussian Quadrature; Gauss Formulae

Let $f \in C[a,b]$, and $p_{n-1}(f)$ be the Lagrange interpolating polynomial. Then the integration error is given as integral of the interpolation error

$$
\begin{aligned}
E_n(f) &= \int_a^b f(t)w(t)dt - \sum_{k=1}^{n} w_k f(t_k) \\
&= \int_a^b w(t)[f(t) - p_{n-1}(f;t)]dt \\
&= \int_a^b w(t)[t_1, \ldots, t_n, t] f \omega_n(t)dt
\end{aligned}
$$

Goal: $E_n(f) = 0$?

If $f \in \mathbf{P}_m$ for some $m \geqslant n$, then $[t_1, \ldots, t_n, t]f \in \mathbf{P}_{m-n}$. I.e.,

$$
\int_a^b w(t)p(t)\omega_n(t)dt = 0, \forall p \in \mathbf{P}_{m-n}
$$

with possibly $m = n, \ldots, 2n-1$. That is, the second condition in the theorem.

(Weighted) Gaussian Quadrature; Gauss Formulae

Definition

A numerical quadrature (3) is called a weighted Gaussian quadrature, if

1. the quadrature points $t_1, \ldots, t_n$ are the n simple roots of an n-th orthogonal polynomial in $L^2_w(a, b)$, i.e.,

$$\pi_n(t_k; w) = 0, \ k = 1, \ldots, n$$

2. the quadrature is interpolatory, i.e.,

$$w_k = \int_a^b w(t) l_k(t) dt = \int_a^b \frac{\pi_n(t; w)}{(t - t_k)\pi_n'(t_k; w)} w(t) dt, \ k = 1, \ldots, n$$

Theorem

A numerical quadrature (3) is a weighted Gaussian quadrature if and only if it has the degree of exactness $2n - 1$.

(Weighted) Gaussian Quadrature; Error

Theorem

Let (3) be a weighted Gaussian quadrature. For any $f \in C^{2n}[a,b]$, there exists $\xi \in [a,b]$ such that

$$\int_a^b f(t)w(t)dt - \sum_{k=1}^n w_k f(t_k) = \frac{f^{(2n)}(\xi)}{(2n)!} \int_a^b w(t) \prod_{k=1}^n (t-t_k)^2 dt$$

Proof. Let $p \in \mathbf{P}_{2n-1}$ be the Hermite interpolation polynomial of f at $t_1, \ldots, t_n$, then the integration error is the integral of the interpolation error; with mean value theorem for weighted integrals; we obtain the error estimate.

Proposition

The coefficients of a weighted Gaussian quadrature are all positive.

Gaussian Quadrature

Gaussian Quadrature

- $w(t) \equiv 1$:

$$\int_{-1}^{1} f(t)dt \approx \sum_{k=1}^{n} w_k f(t_k)$$

- $t_1, \ldots, t_n$ are zeros of n-th Legendre polynomial P_n, $n = 0, 1, \ldots$.
- The coefficients are given by

$$w_k = \frac{2}{(1-t_k)^2[P_n'(t_k)]^2}, \ k = 1, \ldots n$$

- Error: $\frac{f^{(2n)}(\xi)}{(2n)!} \int_{-1}^{1} \prod_{k=1}^{n}(t-t_k)^2 dt = \frac{f^{(2n)}(\xi)}{(2n)!} \int_{-1}^{1} (\frac{2^n n!}{(2n)!})^2 P_n^2(t)dt = f^{(2n)}(\xi)\frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3}$

Gauss-Chebyshev Quadrature

Gauss-Chebyshev Quadrature

- $w(t) = (1-t^2)^{-1/2}$:

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}} dt \approx \sum_{k=1}^{n} w_k f(t_k)$$

- $t_1, \ldots, t_n$ are zeros of n-th Chebyshev polynomial of first kind T_n, $n = 0, 1, \ldots$.
- The coefficients are given by $w_k = \pi/n,\ k = 1, \ldots n$
- Error: $f^{(2n)}(\xi) \frac{\pi}{2^{2n-1}(2n)!}$

Computing Gaussian Quadrature Formula

- Recall the recurrence formula (with $\beta_0 = \int_a^b w(t)dt$):
  $\pi_0(t) = 1, \pi_{-1}(t) = 0,$
  $$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), k = 0, 1, \ldots$$
- n-th order Jacobi matrix for w:
  $$\mathbf{J}_n = \mathbf{J}_n(w) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}$$
- nodes t_k are eigenvalues of $\mathbf{J}_n$: $\mathbf{J}_n \mathbf{v}_k = t_k \mathbf{v}_k, \mathbf{v}_k^T \mathbf{v}_k = 1, k = 1, \ldots .n.$
  weights are: $w_k = \beta_0 v_{k,1}^2, k = 1, \ldots .n.$

Convergence of Sequences of Numerical Quadrature

Theorem

Given a sequence of numerical quadrature

$$\int_a^b f(t)w(t)dt \approx \sum_{k=1}^{n} w_k^{(n)} f(t_k^{(n)}), n = 1, \ldots. \tag{4}$$

Suppose

- $\lim_{n\to\infty} \sum_{k=1}^{n} w_k^{(n)} p(t_k^{(n)}) = \int_a^b w(t)p(t)dt, \forall p \in \mathbf{P}$
- $\sup_{n\geqslant 1} \sum_{k=1}^{n} |w_k^{(n)}| < \infty$

Then

$$\lim_{n\to\infty} \sum_{k=1}^{n} w_k^{(n)} f(t_k^{(n)}) = \int_a^b f(t)w(t)dt, \forall f \in C[a,b].$$

Convergence of Sequences of Numerical Quadrature

Colloary

Given a sequence of numerical quadrature as in (4). Suppose all the coefficients $w_k^{(n)}$ $(k = 1, \ldots, n, n = 1, \ldots)$ are positive. Then

$$\lim_{n\to\infty} \sum_{k=1}^{n} w_k^{(n)} f(t_k^{(n)}) = \int_a^b f(t)w(t)dt, \forall f \in C[a, b].$$

Colloary

For any sequence of weighted Gaussian quadrature as in (4), we have

$$\lim_{n\to\infty} \sum_{k=1}^{n} w_k^{(n)} f(t_k^{(n)}) = \int_a^b f(t)w(t)dt, \forall f \in C[a, b].$$

Gauss-Radau; Gauss-Lobatto

Gauss-Radau Quadrature

- One end point serves as a quadrature point, say a finite, $t_1 = a$.
- $t_2, \ldots, t_n$ are chosen as zeros of $(n-1)$-th orthogonal polynomial $\pi_{n-1}(t; w_a)$ w.r.t. weight $w_a(t) = (t-a)w(t)$.
- Degree of Exactness is $2n-2$.

Gauss-Lobatto Quadrature

- Both end points serve as quadrature points, say a, b finite, $t_1 = a, t_n = b$.
- $t_2, \ldots, t_{n-1}$ are chosen as zeros of $(n-2)$-th orthogonal polynomial $\pi_{n-2}(t; w_{a,b})$ w.r.t. weight $w_{a,b}(t) = (t-a)(b-t)w(t)$.
- Degree of Exactness is $2n-3$.

Method of Interpolation v.s. Method of Undetermined Coefficients; An Example

Obtain a numerical quadrature: $\int_0^1 f(x)dx \approx a_1 f(0) + a_2 f(1)$

- Method of Interpolation:

$$\int_0^1 f(x)dx \approx \int_0^1 p_1(f;0,1;x)dx = \frac{1}{2}(f(0) + f(1))$$

- Method of Undetermined Coefficients: want degree of exactness $= 1$, i.e., exact for $f(x) = 1$ and $f(x) = x$: we have a linear system

$$a_1 + a_2 = 1; a_2 = 2.$$

Hence $a_1 = a_2 = 1/2$.

Richardson Extrapolation

Theorem (Repeated Richardson Extrapolation)

Let $A(h)$ *admits the asymptotic expansion*

$$A(h) = a_0 + a_1 h^{p_1} + a_2 h^{p_2} + \cdots, 0 < p_1 < p_1 < \cdots, h \to 0,$$

and define for some fixed $0 < q < 1$,

$$\begin{aligned} A_1(h) &= A(h), \\ A_{k+1}(h) &= A_k(h) + \frac{A_k(h) - A_k(q^{-1}h)}{q^{-p_k} - 1}, k = 1, 2, \ldots \end{aligned}$$

Then for each $n = 1, 2, \ldots$, $A_n(h)$ *admits an asymptotic expansion*

$$A_n(h) = a_0 + a_n^{(n)} h^{p_n} + a_{n+1}^{(n)} h^{p_{n+1}} + \cdots, h \to 0,$$

with certain coefficients $a_n^{(n)}, a_{n+1}^{(n)}, \ldots$ *not depending on* h.

Composite Trapezoidal Rule

Let $A(h)$ be the composite trapezoidal rule,

$$A(h) = h[\frac{1}{2}f(a) + \sum_{k=1}^{n-1} f(a+kh) + \frac{1}{2}f(b)]$$

Theorem (Euler-Maclaurin Formula)

Assume $f \in C^{2K+1}[a,b]$ *for some* $K > 1$, *then*

$$A(h) = a_0 + a_1 h^2 + a_2 h^4 + \cdots + a_k h^{2K} + O(h^{2K+1}), h \to 0$$

with $a_0 = \int_a^b f(x)dx$ *and* $a_k = \frac{B_{2k}}{(2k)!}[f^{(2k-1)}(b) - f^{(2k-1)}(a)]$,
$k = 1, 2, \ldots, K$, *where* $|B_k| \approx 2\frac{k!}{(2\pi)^k}$ *as* k *(even)* $\to \infty$,
$B_0 = 1, B_2 = \frac{1}{6}, B_4 = \frac{-1}{30}, B_6 = \frac{1}{42}, \cdots, B_1 = \frac{-1}{2}, B_3 = B_5 = \cdots = 0.$

Romberg Integration

Let $A(h)$ be the composite trapezoidal rule,

$$A(h) = h[\frac{1}{2}f(a) + \sum_{k=1}^{n-1} f(a+kh) + \frac{1}{2}f(b)]$$

Romberg Integration

- Let $A_{m,0} = A(q^m h_0)$,

$$A_{m,k} = A_{m,k-1} + \frac{A_{m,k-1} - A_{m-1,k-1}}{q^{-p_k} - 1}, m \geqslant k \geqslant 1,$$

- Choosing $h_0 = b - a, q = 1/2$, $p_k = 2k, k = 1, \ldots, K, p_{K+1} = 2K + 1$

$$A_{m,k} = A_{m,k-1} + \frac{A_{m,k-1} - A_{m-1,k-1}}{4^k - 1}, m \geqslant k \geqslant 1,$$