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

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

a (weighted) numerical quadrature with $t_1, \ldots, t_n$ quadrature points and $w_1, \ldots, w_n$ 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 $k = 0, 1, \ldots, d$.

Numerical Integration; Some Examples

Remark: the degree of exactness of (1) is $\leqslant 2n-1$.

Some examples with $w(t)=1$.

- Trapezoidal rule: degree of exactness is 1?
- Simpson's rule: degree of exactness is 3?

Interpolatory Quadrature

Definition (Interpolatory Quadrature)

The interpolatory quadrature associated with $n+1$ distinct points $t_0, t_1, \dots, t_n$ 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

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

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

Interpolatory Quadrature

Theorem (Characterization of Interpolatory Quqdrature)

Let $t_0, \ldots, t_n$ *be* $n+1$ *distinct points in* $[a, b]$. *A numerical quadrature*

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

is an interpolatory quadrature if and only if its degree of exactness is $\geqslant n$.

Proof.

Newton-Cotes Formula

Newton-Cotes Formula

- $w(t) \equiv 1$, $\{t_0, \ldots, t_n\}$ equally spaced nodes.
- Newton-Cotes formula has degree of exactness $\geqslant n$:

$$\int_a^b f(t)dt = \sum_{k=0}^{n} w_k f(t_k) + E_n(f), \text{ with } w_k = \int_a^b l_k(t)dt \qquad (3)$$

- If $f \in \mathbf{P}_n$, $p_n(f;t) = f(t)$, we see

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

- If it has degree of exactness $\geqslant n$, let $f(t) = l_r(t)$, we see

$$\int_a^b l_r(t)dt = \sum_{k=0}^{n} w_k l_r(t_k) = w_r.$$

The Newton-Cotes Formulas

The Closed Newton-Cotes Formulas

Use nodes $t_i = t_0 + ih, t_0 = a, t_n = b, h = (b-a)/n$:

$$\int_a^b f(t)dt \approx \sum_{i=0}^{n} w_i f(t_i), \text{ with } w_i = \int_{t_0}^{t_n} l_i(t)dt. \tag{4}$$

E.g., $n = 1$ gives the Trapezoidal rule, $n = 2$ gives Simpson's rule.

The Open Newton-Cotes Formulas

Use nodes $t_i = t_0 + ih, t_0 = a + h, t_n = b - h, h = (b-a)/(n+2)$.

E.g., setting $n = 0$ gives the Midpoint rule (Rectangular Rule):
$\int_{t_{-1}}^{t_1} f(x) = 2hf(t_0) + \frac{h^3}{3} f''(\xi)$

Question: what is the difference?

The Newton-Cotes Formulas; Error Formula

Theorem (Error Formula for Newton-Cotes Formula)

Consider a Newton-Cotes Formula (4)*:*

- *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 $\mu_n = \int_a^b t(t-t_0)\cdots(t-t_n)dt < 0.$

- *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 $\nu_n = \int_a^b (t-t_0)\cdots(t-t_n)dt < 0.$

Error Formula; Proof

Lemma

Let $n \geqslant 1$ be even, $h = (b-a)/n$, and $t_k = a + kh$ $(k = 0, \ldots, n)$. Let $\omega_n(t) = (t-t_0)\cdots(t-t_n)$ and $\Omega_n(t) = \int_a^t \omega_n(s)ds$. Then $\Omega_n(a) = \Omega_n(b) = 0$ and $\Omega_n(t) > 0$ for all $t \in (a,b)$.

Proof of Lemma.

Proof of Theorem on Error Formula.

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

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

Proof.