CSC349A Numerical Analysis

Lecture 17

Rich Little

University of Victoria

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Table of Contents I

Introduction

The process of determining areas e.g. area of a circle by inscribed and superscribed polygons. This term is used to avoid confusion with the numeric integration of differential equations.
Problem: approximate the value of

$$\int_a^b f(x)dx$$

where $f(x)$ is such that it cannot be integrated analytically or it is known at only a finite set of points.

The main idea

Approximate $f(x)$ by an interpolating polynomial $P(x)$, and approximate $\int_a^b f(x)dx$ by $\int_a^b P(x)dx$

Suppose $P_n(x)$ is the Lagrange form of the interpolating polynomial:

$$P_n(x) = \sum_{i=0}^{n} L_i(x)f(x_i)$$

then

$$\int_a^b f(x)dx \approx \int_a^b \left[\sum_{i=0}^{n} L_i(x)f(x_i)\right] dx = \sum_{i=0}^{n} \left[\int_a^b L_i(x)dx\right] f(x_i)$$

which is of the form $\sum_{i=0}^{n} a_i f(x_i)$.

Quadrature formula

So, our approximation is of the form

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i).$$

Such an approximation is called a **quadrature formula**, and a_i are the **quadrature coefficients** and x_i are the **quadrature points**, the points at which $f(x)$ is sampled to approximate $\int_a^b f(x)dx$.

Types

Types of quadrature formulas:

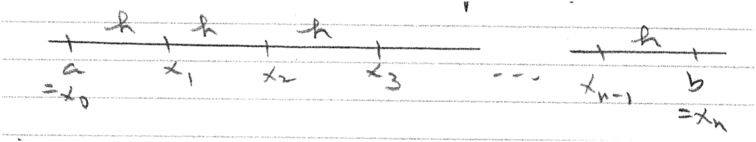
- Newton-Cotes closed
- Newton-Cotes open
- Gaussian (omit)

Any quadrature formula derived by integrating an interpolating polynomial at equally-spaced quadrature points is called a **Newton-Cotes** formula.

Gaussian formulas obtain high accuracy by using optimally-chosen, unequally-spaced quadrature points.

Newton-Cotes closed formulas

Subdivide [a,b] into n subintervals of length $h = \frac{b-a}{n}$.



$$x_{i+1} - x_i = h, x_i = x_0 + ih$$

If $P_n(x)$ interpolates $f(x)$ at $a = x_0, x_1, x_2, \ldots, b = x_n$ and

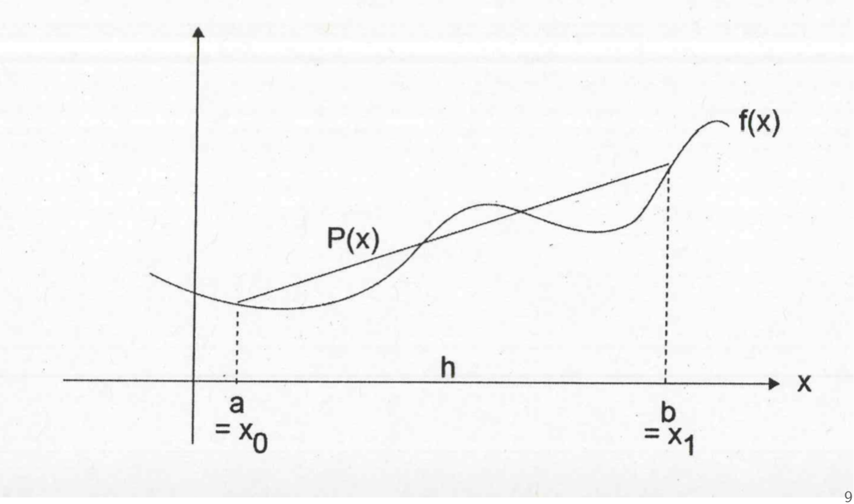
$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx$$

then the resulting quadrature formula is called a **Newton-Cotes** closed formula.

Table of Contents I

Introduction

The case $n = 1$:



Quadrature formula

The quadrature formula for approximating $\int_a^b f(x)dx$ is obtained by integrating P(x):

Quadrature formula continued

Trapezoid rule

This is the **trapezoid rule**.

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(x_0) + f(x_1)]$$

Its error term can be obtained by integrating the error term of the Lagrange form of the interpolating polynomial, which for $n = 1$ is

$$f(x) - P(x) = \frac{f''(\xi)}{2}(x - x_0)(x - x_1)$$

where ξ is in the interval $[a, b]$.

Truncation Error

Integrating this gives:

$$\begin{aligned}\int_a^b f(x)dx - \int_{x_0}^{x_1} P(x)dx &= \int_a^b f(x)dx - \frac{h}{2}[f(x_0) - f(x_1)] \\ &= \int_a^b \frac{f''(\xi)}{2}(x - x_0)(x - x_1)dx \\ &= \frac{f''(\xi)}{2}\int_a^b (x - x_0)(x - x_1)dx\end{aligned}$$

since $f''(\xi)$ is a constant.

Truncation Error

Now, let $t = \frac{x - x_0}{h}$ and integrate $\frac{f''(\xi)}{2} \int_a^b (x - x_0)(x - x_1)dx$ by substitution of variables.

Truncation Error continued

Example 1

Use the Trapezoidal Rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

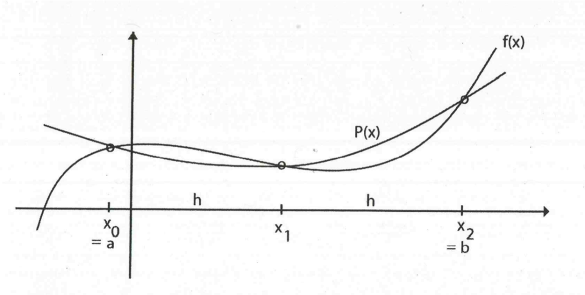
from $a = 0$ to $b = 0.8$ and approximate the absolute error.

Example 1 continued

Qudratic case

For the case $n = 2$ the quadratic interpolating polynomial is:

$$P(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$



Qudrature formula for n=2

As in the case $n = 1$, the quadrature formula for approximating $\int_a^b f(x)dx$ is obtained by integrating $P(x)$: $\int_a^b f(x)dx \approx \int_{x_0}^{x_2} P(x)dx$.
This gives:

$$\int_a^b f(x)dx \approx \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$$

where now $h = \frac{b-a}{2}$. This is called **Simpson's rule** or **Simpson's 1/3 rule**, and its **truncation error** is given by:

$$\int_a^b f(x)dx - \int_{x_0}^{x_2} P(x)dx = -\frac{h^5}{90} f^{(4)}(\xi), \text{ for some } \xi \in [a, b]$$

Example 2

Use the Simpson's $1/3$ Rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$ and approximate the absolute error.

Example 2 continued

Quadrature formula for n=3

The Newton-Cotes closed quadrature formula for $n = 3$ (**Simpson's 3/8 rule**), in which $f(x)$ is approximated by a cubic polynomial that interpolates at four equally-spaced points, is:

$$\int_a^b f(x)dx \approx \frac{3h}{8}(f(x_0)+3f(x_1)+3f(x_2)+f(x_3)), \text{ where } h = \frac{b-a}{3}$$

The truncation error for this is

$$E_t = \frac{-3}{80}h^5 f^{(4)}(\xi)$$

for some $\xi \in [a, b]$.

Example 3

Use the Simpson's 3/8 rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$ and approximate the absolute error.

Example 3 continued

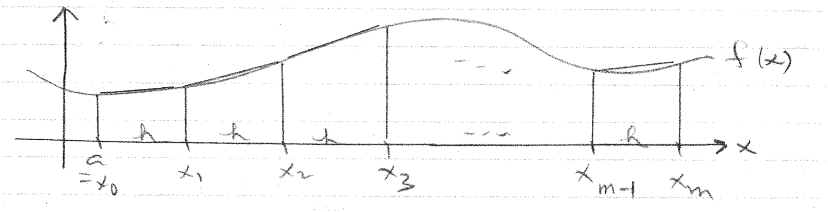
Table of Contents I

Introduction

- Corresponds to sections 21.1.2 and 21.2.2 of the text
- **Objective:** We want the **truncation error** $\rightarrow 0$ as the **number of quadrature points** $\rightarrow \infty$**.**
- Note: this does not happen in general as n, the order of the interpolating polynomial, $\rightarrow \infty$.
- **Solution:** We use composite (multiple-application) quadrature formulas.

Trapezoidal rule

Main idea: for $m \geq 1$, apply a closed N-C formula (with n small) m times on $[a, b]$.
Example: Trapezoidal rule ($n = 1$)
For any $m \geq 1$, let $h = \frac{b-a}{m}$, subdivide $[a, b]$ into m subintervals of length h, and apply the trapezoidal rule on each subinterval.



Composite trapezoidal rule

$$
\begin{aligned}
\int_a^b f(x)dx =& \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{m-1}}^{x_m} f(x)dx \\
\approx& \int_{x_0}^{x_1} P_0(x)dx + \int_{x_1}^{x_2} P_1(x)dx + \cdots + \int_{x_{m-1}}^{x_m} P_{m-1}(x)dx \\
=& \frac{h}{2}\left[f(x_0) + f(x_1)\right] + \frac{h}{2}\left[f(x_1) + f(x_2)\right] + \cdots + \frac{h}{2}\left[f(x_{m-1}) + f(x_m)\right] \\
=& h\left[\frac{f(x_0)}{2} + \sum_{i=1}^{m-1} f(x_i) + \frac{f(x_m)}{2}\right]
\end{aligned}
$$

This is called the composite trapezoial rule.

Truncation Error

$$
\begin{aligned}
E_t &= -\frac{h^3}{12}f''(\xi_1) - \frac{h^3}{12}f''(\xi_2) - \cdots - -\frac{h^3}{12}f''(\xi_m) \\
&= -\frac{h^3}{12}\left[f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_m)\right]
\end{aligned}
$$

where $x_{i-1} \leq \xi_i \leq x_i$.

Truncation Error II

We know that:

$$\min_{1 \le i \le m} f''(\xi_i) \le \frac{f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_m)}{m} \le \max_{1 \le i \le m} f''(\xi_i)$$

If $f''(x)$ is continuous on $[a, b]$, then there exists a value $\mu \in [a, b]$ such that:

$$f''(\mu) = \frac{f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_m)}{m}$$

This is called the intermediate value theorem.

$$E_t = -\frac{h^3}{12}[mf''(\mu)] = -\frac{(b-a)}{12}h^2 f''(\mu)$$

since $h = \frac{b-a}{m}$.

Example 1

Let $m = 2$ and apply the composite Trapezoid rule to numerically integrate the following function from $a = 0$ to $b = 0.8$.

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

Example 1 continued

Important point

$$\lim_{m \to \infty} E_t = \lim_{h \to 0} E_t = 0$$

provided that $f''(x)$ is continuous on $[a, b]$.
(there is no comparable result as $n \to \infty$, where n is the degree of the interpolating polynomial)

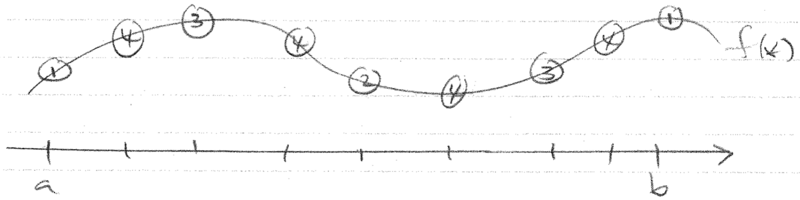
Implementation

Usual implementation of composite trapezoidal:

- Initialize $m = 1$
- Repeatedly double m (m=1,2,4,8,16,32,...)
- Until two consecutive approximations are sufficiently close

Reusing function evaluations

The reason for using these values of m is that they permit re-use of the function evaluations from previous evaluations i.e all values $f(x_i)$ computed for $m = k$ can be re-used for $m = 2k$.



Composite Simpson's Rule

- Each application of Simpson's rule requires 2 subintervals on the interval of integration and 3 quadrature points.
- Thus, m applications of Simpson's rule on $[a, b]$ require that $[a, b]$ be subdivided into $2m$ subintervals using $2m + 1$ quadrature points.
- Each subinterval then is of length

$$h = \frac{b - a}{2m}$$

Composite Simpson's Rule II

Thus, at the *jth* subinterval we have the three quadrature points x_{2j-2}, x_{2j-1}, and x_{2j}, and

$$\int_{x_{2j-2}}^{x_{2j}} f(x)dx \approx \frac{h}{3}\left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\right]$$

When $m = 1$ (regular Simpson's rule) we have $2(1) + 1 = 3$ quadrature points and 2 subintervals each of length $h = \frac{b-a}{2}$.

Composite Simpson's Rule ($m = 2$)

When $m = 2$, we apply Simpson's rule twice. We need $2(2) + 1 = 5$ quadrature points to create 4 subintervals each of length $h = \frac{b-a}{4}$.

Here,

$$\int_a^b f(x)dx$$
$$\approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right]$$
$$= \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)\right]$$

General Composite Simpson's Rule

In general, when $m \geq 1$, the composite Simpson's rule approximation is

$$\begin{aligned}
&\int_a^b f(x)dx \\
&\quad \approx \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \\
&\qquad \cdots + 2f(x_{2m-2}) + 4f(x_{2m-1}) + f(x_{2m})] \\
&\quad = \frac{h}{3}\left[f(x_0) + 4\sum_{j=1}^{m} f(x_{2j-1}) + 2\sum_{j=1}^{m-1} f(x_{2j}) + f(x_{2m})\right]
\end{aligned}$$

Truncation Error

$$
\begin{aligned}
E_t &= -\frac{h^5}{90} f^{(4)}(\xi_1) - \frac{h^5}{90} f^{(4)}(\xi_2) - \cdots - -\frac{h^5}{90} f^{(4)}(\xi_m) \\
&= -\frac{h^5}{90}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_2) + \cdots + f^{(4)}(\xi_m)\right] \\
&= -\frac{h^5}{90}[m f^{(4)}(\mu)]
\end{aligned}
$$

where $a \leq \mu \leq b$ and $f^{(4)}(x)$ is continous. So,

$$
E_t = -\frac{(b-a)h^4}{180} f^{(4)}(\mu)
$$

since $h = \frac{b-a}{2m}$.

Example 2

Let $m = 2$ and apply the composite Simpson's rule to numerically integrate the following function from $a = 0$ to $b = 0.8$.

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

Example 2 continued