Part 6. Numerical Differentiation and Integration
Chapter 21. Newton-Cotes Integration Formulas

Lecture 20

Simpson's Rule

21.2

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Motivation

- More accurate estimate of an integral is obtained if a high-order polynomial is used to connect the points.

- The formulas that result from taking the integrals under such polynomials are called *Simpson's rules*.

Simpson's 1/3rd Rule

Trapezoidal Rule:

approximating integrand by a 1st order polynomial

Simpson's 1/3rd Rule:

approximating integrand by a 2nd order polynomial

$$I = \int_a^b f(x)\ dx \approx \int_a^b (a_0 + a_1 x + a_2 x^2)\ dx$$

Simpson's 1/3rd Rule

To find a_0, a_1 and a_2 three points are chosen:

Upper limit	Midpoint	Lower limit
$(a, f(a)),$	$\left(\frac{a+b}{2}, f\left(\frac{a+b}{2}\right)\right),$	$(b, f(b))$

$$f(a) = f_2(a) = a_0 + a_1 a + a_2 a^2$$

$$f\left(\frac{a+b}{2}\right) = f_2\left(\frac{a+b}{2}\right) = a_0 + a_1\left(\frac{a+b}{2}\right) + a_2\left(\frac{a+b}{2}\right)^2$$

$$f(b) = f_2(b) = a_0 + a_1 b + a_2 b^2$$

Simpson's 1/3rd Rule

Solving the previous equations for a_0, a_1 and a_2 give

$$a_0 = \frac{a^2 f(b) + abf(b) - 4abf\left(\frac{a+b}{2}\right) + abf(a) + b^2 f(a)}{a^2 - 2ab + b^2}$$

$$a_1 = -\frac{af(a) - 4af\left(\frac{a+b}{2}\right) + 3af(b) + 3bf(a) - 4bf\left(\frac{a+b}{2}\right) + bf(b)}{a^2 - 2ab + b^2}$$

$$a_2 = \frac{2\left(f(a) - 2f\left(\frac{a+b}{2}\right) + f(b)\right)}{a^2 - 2ab + b^2}$$

Simpson's 1/3rd Rule

$$I \approx \int_a^b f_2(x)\,dx$$

$$= \int_a^b \left(a_0 + a_1 x + a_2 x^2\right) dx$$

$$= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} \right]_a^b$$

$$= a_0(b-a) + a_1 \frac{b^2 - a^2}{2} + a_2 \frac{b^3 - a^3}{3}$$

Substituting values of a_0, a_1, a_2 give

Simpson's 1/3rd Rule

$$\int_a^b f_2(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

The interval [a, b] was broken into 2 segments. Then, the segment width is

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

$$\int_a^b f_2(x)\ dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

Because the above form has 1/3 in its formula, it is called Simpson's 1/3rd Rule.

Multiple-Section Simpson's 1/3rd Rule

Multiple-Section Simpson's 1/3rd Rule

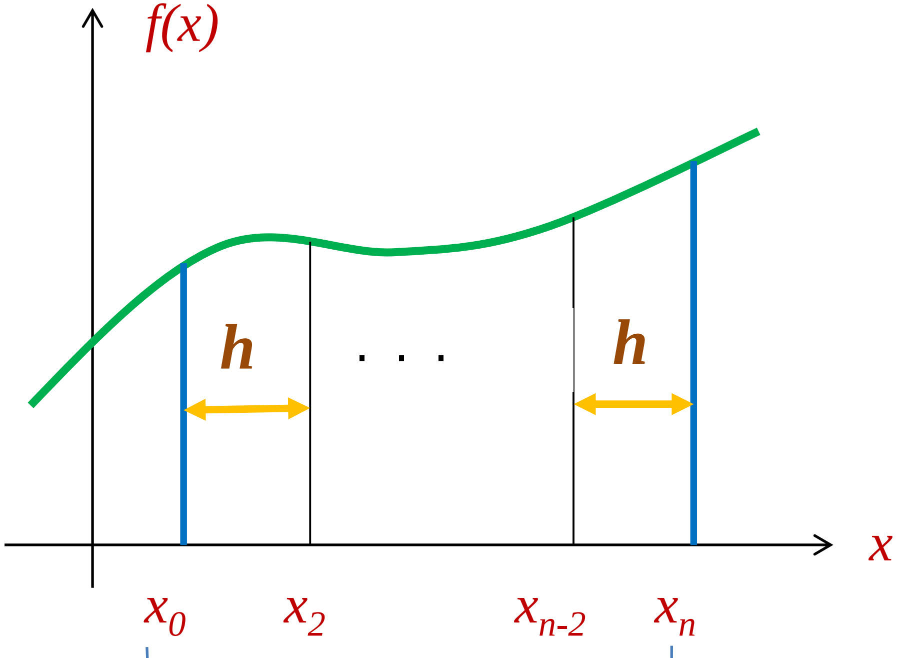
Interval [a, b] divided into **n** equal sections

Simpson's 1/3rd Rule applied repeatedly over every two section

Segment width

$$h = \frac{b-a}{n}$$

$$\int_a^b f(x)\ dx = \int_{x_0}^{x_n} f(x)\ dx$$



$$x_0 = a \qquad x_n = b$$

Multiple-Section Simpson's 1/3rd Rule

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \ldots\ldots + \int_{x_{n-4}}^{x_{n-2}} f(x)dx + \int_{x_{n-2}}^{x_n} f(x)dx$$

Simpson's 1/3rd Rule application over each interval:

$$\int_a^b f(x)dx = (x_2 - x_0)\left[\frac{f(x_0)+4f(x_1)+f(x_2)}{6}\right] + \ldots$$

$$+ (x_4 - x_2)\left[\frac{f(x_2)+4f(x_3)+f(x_4)}{6}\right] + \ldots\ldots\ldots$$

$$+ (x_n - x_{n-2})\left[\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}\right]$$

$$x_i - x_{i-2} = 2h \qquad\qquad i = 2, 4, \ldots, n$$

Multiple-Section Simpson's 1/3rd Rule

$$\int_a^b f(x)dx = 2h\left[\frac{f(x_0)+4f(x_1)+f(x_2)}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_2)+4f(x_3)+f(x_4)}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_{n-4})+4f(x_{n-3})+f(x_{n-2})}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}\right]$$

Multiple-Section Simpson's 1/3rd Rule

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(x_0)+4\left\{f(x_1)+f(x_3)+\ldots+f(x_{n-1})\right\}+\ldots\right]$$

$$\ldots+2\left\{f(x_2)+f(x_4)+\ldots+f(x_{n-2})\right\}+f(x_n)\}]$$

$$=\frac{h}{3}\left[f(x_0)+4\sum_{\substack{i=1\\ i=odd}}^{n-1} f(x_i)+2\sum_{\substack{i=2\\ i=even}}^{n-2} f(x_i)+f(x_n)\right]$$

$$=\frac{b-a}{3n}\left[f(x_0)+4\sum_{\substack{i=1\\ i=odd}}^{n-1} f(x_i)+2\sum_{\substack{i=2\\ i=even}}^{n-2} f(x_i)+f(x_n)\right]$$

Error in the Multiple-Section Simpson's 1/3rd Rule

True error is proportional to:

$$E_t \propto \frac{1}{n^4}$$

If number of segments are doubles the true error is decreased 16 times

Example 1. Find $\int_0^2 x^4 dx$ using Simpson's 1/3 rule with

n = 8

i	*x*	*f (x)*
0		
1		
2		
3		
4		
5		
6		
7		
8		

Error in the Multiple-Section Simpson's 1/3rd Rule

Error in the Multiple-Section Simpson's 1/3rd Rule

The true error in a single application of the rule is:

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\zeta), \quad a < \zeta < b$$

In multiple-section rule is the sum of the errors in each application of the rule:

$$E_t = \sum_{i=1}^{\frac{n}{2}} E_i \qquad = -\frac{h^5}{90} \sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i) \quad = -\frac{(b-a)^5}{90n^5} \sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)$$

$$E_t = -\frac{(b-a)^5}{90n^4} \frac{\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)}{n}$$

Error in the Multiple-Section Simpson's 1/3rd Rule

The term $\dfrac{\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)}{n}$ is an approximate average value of

$$f^{(4)}(x),\ a < x < b \qquad E_t = -\frac{(b-a)^5}{90n^4}\overline{f}^{(4)}$$

where

$$\overline{f}^{(4)} = \frac{\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)}{n}$$

If interested, the complete derivation of truncation error in Simpson's 1/3 rule can be found in a separate note on the course website.

Part 6. Numerical Differentiation and Integration
Chapter 22. Integration of Equations

Lecture 21

Romberg Integration & Gauss Quadrature

22.2, 22.4

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Forms of Functions in Numerical Integration

- They are in 2 forms:

A Table of Values

- We are restricted by the number of points that are given.

A Function

- We can produce as many values of $f(x)$ as required to get acceptable accuracy.

Techniques for Integration of Functions

We focus on 2 techniques designed to analyze functions:

- Romberg Integration
- Gauss Quadrature

Romberg Integration

- Is based on recursive application of the trapezoidal rule to attain efficient numerical integrals of functions.

- Error correction technique is used to improve the result of numerical integration

Richardson's Extrapolation

- Uses two estimates of an integral to compute a third and more accurate approximation.

Richardson's Extrapolation by Trapezoidal Rule

- It uses two estimates of an integral to compute a third and more accurate approximation.

$$I_{exact} = I_{trapez} + E_t \qquad\qquad E_t \propto \frac{1}{n^2}$$

- Estimate integral by using n segment trapezoidal rule
- Estimate integral by using 2n-segment trapezoidal rule
- Knowledge of change of E_t with n help us to better estimate integral by two other estimates found by n and 2n segments

Example. Richardson's extrapolation. Using approximate integral values using different segments of trapezoidal rule (1 to 8) given for the following function representing position of a rocket:

$$x = \int_{8}^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100\,t} \right] - 9.8\,t \right) dt$$

find a better estimate using Richardson's extrapolation.

Romberg Integration

$$I_{Romberg} = \frac{4I_{trap,2} - I_{trap,1}}{3}$$

Using n and 2n segment Trapezoid

$$I_{Romberg} = \frac{4I_{trap,4} - I_{trap,2}}{3}$$

Using 2n and 4n

$$I_{Romberg} = \frac{4I_{trap,8} - I_{trap,4}}{3}$$

Using 4n and 8n

$$I_{trap} = \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f_i + f(b)\right]$$

Example. Robmerg Integration.

$$\int_0^2 x^4 dx$$

n	h	I (trapezoid)
4		
8		
16		

Numerical Integration Notes (Trapezoid, Simpson's, Romberg)

All methods (trapezoidal, Simpson's, Romberg) use <u>evenly spaced functional values</u>

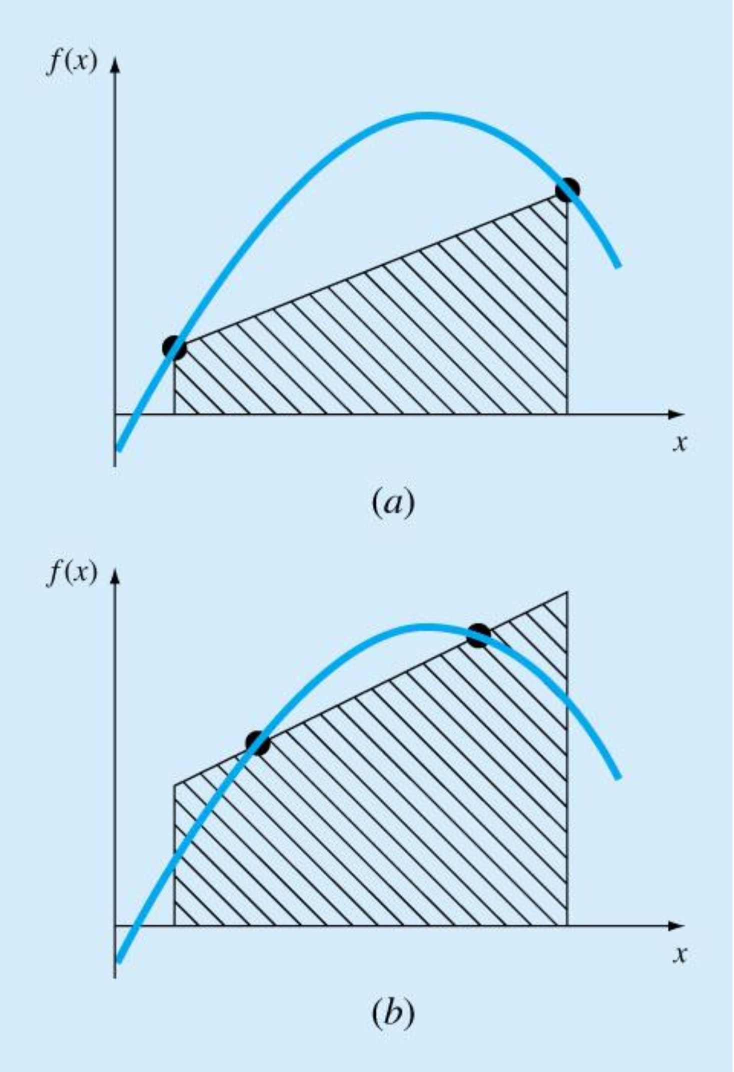
- Trapezoidal rule: base point fixed
- Position point such that area under the curve is almost same as area of trapezoid area
- For less error → Gauss Quadrature can be used

Gauss Quadrature

Gauss Quadrature

Features:

- Instead of two fixed points
- Choose points that balance positive and negative errors



Gauss Quadrature: 2-Point

The extension of Trapezoidal Rule is called the two-point Gauss Quadrature Rule or Gaussian Quadrature Rule

Method of undetermined coefficient for trapezoidal rule

is used for Gauss quadrature

$$I = \int_a^b f(x)dx \quad \approx c_1 f(x_1) + c_2 f(x_2)$$

Gauss Quadrature: 2-Point

- Straight line pass through 2 intermediate points
- 4 unknowns : Two coefficient and two x-values in points 1 and 2.
- Third-order polynomial can be used to approximate f(x) and solve for coefficients and x-values

(see written notes)

Recall: Trapezoidal Rule

Trapezoidal Rule could be developed by the method of undetermined coefficients:

$$I = \int_a^b f(x)dx \approx c_1 f(a) + c_2 f(b)$$

$$= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$

What if : the arguments of the function are not predetermined as a and b but as unknowns x_1 and x_2 ?

$$I = \int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$$

Gauss Quadrature

The four unknowns x_1, x_2, c_1 and c_2 are found by assuming that the formula gives exact results for integrating a general third order polynomial,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

$$\int_a^b f(x)dx = \int_a^b \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right)dx$$

$$= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} + a_3 \frac{x^4}{4}\right]_a^b$$

$$= a_0(b-a) + a_1\left(\frac{b^2 - a^2}{2}\right) + a_2\left(\frac{b^3 - a^3}{3}\right) + a_3\left(\frac{b^4 - a^4}{4}\right)$$

Gauss Quadrature

$$\int_a^b f(x)dx = c_1\left(a_0 + a_1x_1 + a_2x_1^{\ 2} + a_3x_1^{\ 3}\right) + c_2\left(a_0 + a_1x_2 + a_2x_2^{\ 2} + a_3x_2^{\ 3}\right)$$

Equating Equations the two previous two expressions yield

$$a_0(b-a) + a_1\left(\frac{b^2-a^2}{2}\right) + a_2\left(\frac{b^3-a^3}{3}\right) + a_3\left(\frac{b^4-a^4}{4}\right)$$

$$= c_1\left(a_0 + a_1x_1 + a_2x_1^{\ 2} + a_3x_1^{\ 3}\right) + c_2\left(a_0 + a_1x_2 + a_2x_2^{\ 2} + a_3x_2^{\ 3}\right)$$

$$= a_0(c_1 + c_2) + a_1(c_1x_1 + c_2x_2) + a_2\left(c_1x_1^{\ 2} + c_2x_2^{\ 2}\right) + a_3\left(c_1x_1^{\ 3} + c_2x_2^{\ 3}\right)$$

Gauss Quadrature

Since the constants a_0, a_1, a_2, a_3 are arbitrary

$$b - a = c_1 + c_2$$

$$\frac{b^2 - a^2}{2} = c_1 x_1 + c_2 x_2$$

$$\frac{b^3 - a^3}{3} = c_1 {x_1}^2 + c_2 {x_2}^2$$

$$\frac{b^4 - a^4}{4} = c_1 {x_1}^3 + c_2 {x_2}^3$$

Gauss Quadrature

The previous four simultaneous nonlinear Equations have only one acceptable solution,

$$x_1 = \left(\frac{b-a}{2}\right)\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2} \qquad x_2 = \left(\frac{b-a}{2}\right)\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}$$

$$c_1 = \frac{b-a}{2} \qquad c_2 = \frac{b-a}{2}$$

Gauss Quadrature

$$\int_a^b f(x)\, dx \approx c_1 f\left(x_1\right)+c_2 f\left(x_2\right)$$

$$=\frac{b-a}{2} f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right)+\frac{b+a}{2}\right)+\frac{b-a}{2} f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right)+\frac{b+a}{2}\right)$$

Note that this derivation is more general with integral boundaries of a to b

For simplicity the integration limits can be converted (e.g. to -1 to 1 , used in textbook)

Higher Point Gauss Quadrature (n-point)

Gauss Quadrature: n-points

$$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$

three-point Gauss Quadrature

The coefficients c_1, c_2, and c_3, and the functional arguments x_1, x_2, and x_3

Unknowns are found by assuming the formula gives exact expressions for integrating a fifth order polynomial

$$\int_a^b \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5\right)dx$$

General n-point rules would approximate the integral

$$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + \ldots\ldots\ldots + c_n f(x_n)$$

Coefficients c and function arguments x used in Gauss Quadrature

In textbook, coefficients and arguments given for n-point Gauss Quadrature are given for integrals:

$$\int_{-1}^{1} g(x)dx \cong \sum_{i=1}^{n} c_i g(x_i)$$

Points	**Coefficients**	**Function Arguments**
2	c_1 = 1.000000000 c_2 = 1.000000000	x_1 = -0.577350269 x_2 = 0.577350269
3	c_1 = 0.555555556 c_2 = 0.888888889 c_3 = 0.555555556	x_1 = -0.774596669 x_2 = 0.000000000 x_3 = 0.774596669
4	c_1 = 0.347854845 c_2 = 0.652145155 c_3 = 0.652145155 c_4 = 0.347854845	x_1 = -0.861136312 x_2 = -0.339981044 x_3 = 0.339981044 x_4 = 0.861136312

Coefficients c and function arguments x used in Gauss Quadrature

Points	Coefficients	Function Arguments
5	c_1 = 0.236926885 c_2 = 0.478628670 c_3 = 0.568888889 c_4 = 0.478628670 c_5 = 0.236926885	x_1 = -0.906179846 x_2 = -0.538469310 x_3 = 0.000000000 x_4 = 0.538469310 x_5 = 0.906179846
6	c_1 = 0.171324492 c_2 = 0.360761573 c_3 = 0.467913935 c_4 = 0.467913935 c_5 = 0.360761573 c_6 = 0.171324492	x_1 = -0.932469514 x_2 = -0.661209386 x_3 = -0.2386191860 x_4 = 0.2386191860 x_5 = 0.661209386 x_6 = 0.932469514