Romberg Integration and Gaussian Quadrature

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Overview

We discuss two methods for integration.

Romberg Integration

- Romberg integration method is an extrapolation formula of the Trapezoidal rule for integration. It provides a better approximation of the integral by reducing the "true error".
- Two estimates of an integral are used to compute a third integral, the third integral is more accurate than the previous integrals.

Gaussian Quadrature

- The **Gaussian quadrature formulas**, are based on defining $f_n(x)$ using polynomial interpolation at **carefully selected node points** that need not be evenly spaced.

Romberg Integration

The integral

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

is approximated using the composite Trapezoidal rule with step size

$$h_k = \frac{b-a}{2^k}$$

where k is a nonnegative integer.

For each k, Richardson extrapolation is used $k-1$ times to previously computed approximations in order to improve the order of accuracy as much as possible.

More precisely, suppose that we compute approximate values $I(h)$ and $I(h/2)$ to the integral, using the composite Trapezoidal rule with two difference subintervals of widths h and $h/2$ respectively, where $h = b - a$.

If we denote the exact value of the integral by $I(f)$, then we have

$$I(h) = I(f) - \frac{(b-a)}{12} h^2 f''(\eta) \quad \text{for some } \eta \in [a, b]$$

and

$$I\left(\frac{h}{2}\right) = I(f) - \frac{(b-a)}{12} \left(\frac{h}{2}\right)^2 f''(\xi) \quad \text{for some } \xi \in [a, b].$$

It is reasonable to assume that the quantitites $f''(\eta)$ and $f''(\xi)$ are very nearly the same.

Since $f''(\eta) = f''(\xi)$, we get

$$I(h) = I(f) - \frac{(b-a)}{12} h^2 f''(\xi)$$

and

$$I\left(\frac{h}{2}\right) = I(f) - \frac{(b-a)}{12}\left(\frac{h}{2}\right)^2 f''(\xi).$$

Solving for $I(f)$ we get the value of $I(f)$, which we denote by $I(h, h/2)$, is an improved approximation given by

$$I(h, h/2) = I\left(\frac{h}{2}\right) + \left[\frac{I\left(\frac{h}{2}\right) - I(h)}{3}\right].$$

In a similar way we get

$$I\left(\frac{h}{2}, \frac{h}{4}\right) = I\left(\frac{h}{4}\right) + \left[\frac{I\left(\frac{h}{4}\right) - I\left(\frac{h}{2}\right)}{3}\right].$$

Table

With the notations defined above the following table can be formed.

$I(h)$			
$I\left(\frac{h}{2}\right)$	$I\left(h, \frac{h}{2}\right)$		
$I\left(\frac{h}{4}\right)$	$I\left(\frac{h}{2}, \frac{h}{4}\right)$	$I\left(h, \frac{h}{2}, \frac{h}{4}\right)$	
$I\left(\frac{h}{8}\right)$	$I\left(\frac{h}{4}, \frac{h}{8}\right)$	$I\left(\frac{h}{2}, \frac{h}{4}, \frac{h}{8}\right)$	$I\left(h, \frac{h}{2}, \frac{h}{4}, \frac{h}{8}\right)$

The computations can be stopped when two successive values are sufficiently close to each other.

This method, due to L.F. Richardson, is called the **deferred approach to the limit** and the systematic tabuation of this is called **Romberg Integration**.

Degree of Precision

A numerical integration formula $\tilde{I}(f)$ that approximates $I(f)$ is said to have **degree of precision** m if

1. $\tilde{I}(f) = I(f)$ for all polynomials $f(x)$ of degree $\leq m$.
2. $\tilde{I}(f) \neq I(f)$ for some polynomial $f(x)$ of degree $m+1$.

The degrees of precision of Trapezoidal and Simpson's $\frac{1}{3}$-rule are 1 and 3 respectively.

Gaussian Quadrature

For integrals in which the integrand has some kind of bad behavior, for example, an infinite value at some point, we often will consider the integrand in the form

$$I(f) = \int_a^b w(x)\ f(x)\ dx.$$

The bad behavior is assumed to be located in $w(x)$, called the **weight function**, and the function $f(x)$ will be assumed to be well-behaved.

For example, consider evaluating

$$\int_0^1 (\log x)\ f(x)\ dx$$

for arbitrary continuous functions $f(x)$.

Most numerical integration formulas are based on defining $f_n(x)$ in

$$I_n(f) = \int_a^b f_n(x)\ dx = I(f_n)$$

by using polynomials or piecewise polynomial interpolation. Formulas using such interpolation with evenly spaced node points are derived and discussed below.

The **Gaussian quadrature formulas**, are based on defining $f_n(x)$ using polynomial interpolation at carefully selected node points that need not be evenly spaced.

Romberg integration is superior to Simpson's rule, but **Gaussian quadrature is still more rapidly convergent.**

The composite trapezoidal and Simpson rules are based on using a **low-order polynomial** approximation of the integrand $f(x)$ on subintervals of decreasing size.

We investigate a class of methods that use polynomial approximations of $f(x)$ of **increasing degree**.

The resulting integration formulas are extremely accurate in most cases, and they should be considered seriously by anyone faced with many integrals to evaluate.

We discussed some integration formulae which require values of the function at equally-spaced points of the interval.

Gauss derived a formula which uses nodes with different spacing and gives better accuracy.

Gauss' formula is expressed in the form

$$\int_{-1}^{1} f(x)\ dx = \sum_{j=1}^{n} w_j f(x_j)$$

where w_j and x_j are called the **weights** and **nodes**, respectively.

The weights and nodes are to be determined to make the error

$$E_n(f) = \int_{-1}^{1} f(x)\ dx - \sum_{j=1} w_j f(x_j)$$

equal zero for as high a degree polynomial $f(x)$ as possible.

To derive equations for the nodes and weights, we first note that

$$E_n(a_0 + a_1 x + \cdots + a_m x^m) = a_0 E_n(1) + a_1 E_n(x) + \cdots + a_m E_n(x^m).$$

Thus $E_n(f) = 0$ for every polynomial of degree $\leq m$ if and only if

$$E_n(x^i) = 0 \qquad i = 0, 1, \ldots, m.$$

Case : 1 $n = 1$. Since there are two parameters, w_1 and x_1, we consider requiring

$$E_n(1) = 0 \qquad E_n(x) = 0.$$

This gives

$$\int_{-1}^{1} 1 \; dx - w_1 = 0 \qquad \int_{-1}^{1} x dx - w_1 x_1 = 0.$$

This implies $w_1 = 2$ and $x_1 = 0$. Thus the formula becomes

$$\int_{-1}^{1} f(x) \; dx = 2f(0)$$

which the **midpoint rule**.

Case : 2 $n = 2$. There are four parameters, w_1, w_2, x_1 and x_2, and thus we put four constraints on these parameters

$$E_n(x^i) = \int_{-1}^{1} x^i \, dx - \left[w_1 x_1^i + w_2 x_2^i \right] = 0 \qquad i = 0, 1, 2, 3.$$

Thus

$$\begin{aligned} w_1 + w_2 &= 2 \\ w_1 x_1 + w_2 x_2 &= 0 \\ w_1 x_1^2 + w_2 x_2^2 &= 2/3 \\ w_1 x_1^3 + w_2 x_2^3 &= 0. \end{aligned}$$

These equations lead to the unique formula

$$\int_{-1}^{1} f(x) \, dx = f\left(\frac{-\sqrt{3}}{3} \right) + f\left(\frac{\sqrt{3}}{3} \right)$$

which has **degree of precision three.** Note that Simpson's rule users **three nodes** to attain the same degree of precision.

Case : 3

For a general n there are $2n$ free parameters

$$x_1, x_2, \ldots, x_n, w_1, w_2, \ldots, w_n,$$

there is a formula

$$\int_{-1}^{1} f(x)\ dx = \sum_{j=1}^{n} w_j f(x_j)$$

that uses n nodes and gives a degree of precision of $2n-1$.

The equations to be solved are

$$E_n(x^i) = 0 \qquad i = 0, 1, 2, \ldots, 2n-1.$$

These are **nonlinear equations**, and **their solvabiity is not at all obvious**.

Gauss-Legendre Quadrature

This method uses roots (called **Gauss points**) of Legendre polynomials to locate the points at which the integrand is evaluated.

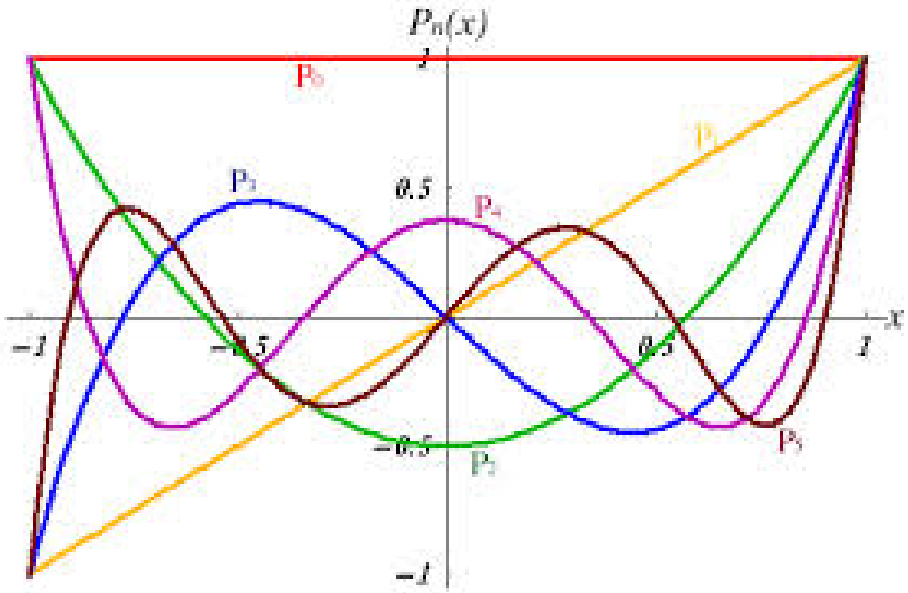
Legendre polynomials

Consider the recursive relation with $P_0(x) = 1$ and $P_1(x) = x$

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

The first five Legendre polynomials are

$$\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= \frac{3x^2 - 1}{2} \\
P_3(x) &= \frac{5x^3 - 3x}{2} \\
P_4(x) &= \frac{35x^4 - 30x^2 + 3}{8} \\
P_5(x) &= \frac{63x^5 - 70x^3 + 15x}{8}
\end{aligned}$$



Example

Consider the Legendre polynomial $P_n(x)$ of degree n.

The roots of $P_n(x)$ are denoted by $x_1, x_2, \ldots, x_n$.

The corresponding weights w_i $(1 \leq i \leq n)$ are given by

$$w_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \, dx.$$

For instance, we solve $P_4(x) = \frac{35x^4 - 30x^2 + 3}{8} = 0$ which gives the four Gauss nodes

$$x_i = \pm \left(\frac{15 \pm 2\sqrt{30}}{35} \right)^{1/2}.$$

The nodes and weights are extensively tabulated for different values of n.

We list below, in the following table, the nodes and weights for Gaussian integration, for values of n upto $n = 5$.

degree n	**nodes** u_i	**weights** w_i
2	$-0.577350269189625 7$	1
2	$0.577350269189625 7$	1
3	0	0.888888888888888
3	$-0.774596669241483 4$	0.555555555555556
3	$0.774596669241483 4$	0.555555555555556
4	$-0.339981043584856 3$	$0.652145154862546 1$
4	$0.339981043584856 3$	$0.652145154862546 1$
4	$-0.861136311594052 6$	$0.347854845137453 8$
4	$0.861136311594052 6$	$0.347854845137453 8$
5	0	0.568888888888889
5	$-0.538469310105683 1$	$0.478628670499366 5$
5	$0.538469310105683 1$	$0.478628670499366 5$
5	$-0.906179845938664 0$	$0.236926885056189 1$
5	$0.906179845938664 0$	$0.236926885056189 1$

Changing Limits

We discussed to evaluate the integral in the form $\int_{-1}^{1} f(x)\ dx$.

How to integrate $f(x)$ over any interval of the form $[a, b]$?

The transformation

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

changes the limits a and b to -1 and 1 respectively.

Hence

$$\int_a^b f(x)\ dx = \int_{-1}^{1} f\left(\frac{2x-a-b}{b-a}\right)\left(\frac{b-a}{2}\right)\ du.$$

The transformation $x = \frac{u+1}{2}$ changes the integral

$$\int_0^1 x\ dx \qquad \text{into} \qquad \frac{1}{4}\int_{-1}^{1}(u+1)\ du.$$

References

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- Kendall E. Atkinson, "*An Introduction to Numerical Analysis*", John Wiley & Sons, Delhi, 1989.
- S.S. Sastry, *Introductory Methods of Numerical Analysis*, Fourth Edition, Prentice-Hall, India.