Introduction to Computational Mathematics (AMATH 242/CS 371)

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Numerical Integration

Our objective in this chapter is calculating $\int_a^b f(x)dx$ which is equivalent to finding the area under $f(x)$. If the area is not regular then integral can be obtained using Riemann Sum:

$$R_n = \sum_{i=0}^{n} (x_i - x_{i-1}) f(c_i)$$

where, $a = x_0 < x_1 < \cdots < x_n = b$ and $c_i \in [x_{i-1}, x_i],\ i = 0, 1, \cdots, n$. If we divide the area under the curve into many rectangles (n is large enough) i.e. $h_n = \max\{(x_i - x_{i-1}),\ i = 0, \cdots, n\}$ approaches zero and $\lim_{n\to\infty} R_n = R$ (R is finite), then f(x) is Riemann integrable on [a,b] and $\int_a^b f(x)dx = R$.

Numerical Integration

Riemann integral on a closed interval **exists** if f(x) is a bounded function with a finite number of discontinuity.

Problems in solving the integral by Riemann Sum: For large *n* which gives the accurate solution, f(x) should be evaluated at many points, i.e. computational work is huge. Note that desired accuracy is obtained if points are chosen carefully.

It seems, finding efficient methods that produce high accuracy at relatively low cost is essential.

Usefulness of integration is not limited to the application in geometry. It includes:

- Integral transforms such as Laplace and Fourier transformations
- Special functions of applied mathematics and mathematical physics have integral representation such as gamma, beta and error function
- Integral equations and variational method

Numerical Quadrature:

We can find $\int_a^b f(x)dx$ analytically by finding an antiderivative F such that $F'(x) = f(x)$ then using the **Fundamental Theorem of Calculus** $\int_a^b f(x)dx = F(b) - F(a)$. For some functions, integral can not be evaluated in such a closed form e.g. for $f(x) = e^{-x^2}$. So, we are often forced to employ numerical methods to evaluate definite integrals approximately. The numerical approximation of definite integrals is known as **numerical quadrature**.

In approximating integrals, we use the concept of Riemann sums that defines the integral :

The integral will be approximated by a weighted sum of integrand values at a finite number of sample points in the interval of integration:

$$I(f) = \int_a^b f(x)dx \approx Q_n(f) = \sum_{i=0}^{n} w_i f(x_i)$$

x_i are nodes and w_i are called weights or coefficients. Main objective is choosing the nodes and weights so that we obtain a desired level of accuracy at a reasonable computational cost in terms of the number of integrand evaluations required.

Quadrature rules can be derived using polynomial interpolation. If $f(x_i),\ i = 0, \cdots, n$ are given, then the polynomial of degree n that interpolates x_i can be determined, and the integral of the interpolant is taken as an approximation to the integral of the original function.

In practice, interpolating polynomial is not to be determined explicitly each time to evaluate a particular integral. Instead polynomial interpolation is used to determine the nodes and weights for a given quadrature rules.

Numerical Integration

One approach for finding nodes and weights is called method of undetermined coefficients. In this method, the rule integrates the first n polynomial basis function exactly, which results in a system of n equations in n unknown. For example, with the monomial basis this strategy yields

$$w_0 \times 1 + \cdots + w_n \times 1 = \int_a^b 1dx = b - a$$

$$w_0 \times x_0 \cdots + w_n \times x_n = \int_a^b xdx = \frac{1}{2}(b^2 - a^2)$$

$$\vdots$$

$$w_0 \times x_0^{n-1} \cdots + w_n \times x_n^{n-1} = \int_a^b x^{n-1}dx = \frac{1}{n}(b^n - a^n)$$

which is equal to

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_0 & x_1 & \cdots & x_n \\ \vdots & \vdots & \ddots & \\ x_0^{n-1} & x_1^{n-1} & \cdots & x_n^{n-1} \end{pmatrix} \times \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} b-a \\ \frac{1}{2}(b^2-a^2) \\ \vdots \\ \frac{1}{n}(b^n-a^n) \end{pmatrix}$$

Solving the above linear system gives weights.
Questions:
1- How to find nodes?$\Longrightarrow$ use Newton-Cotes quadrature
2- Is there any alternative to find weights without solving a linear system?
$\Longrightarrow$ yes, see the next slide.

Newton-Cotes Quadrature: The simplest placement of nodes for a quadrature rule is to choose equally spaced points in [a,b] which is the defining property of Newton-Cotes quadrature: $x_i = a + ih, \ i = 0, \cdots, n$ in which $h = \dfrac{b-a}{n}$.
To find weights without solving the linear system, we use Lagrange interpolating polynomial: $y_n(x) = \sum_{i=0}^{n} f_i L_i(x)$

$$\begin{aligned}\int_a^b f(x)dx &= \int_a^b \sum_{i=0}^{n} f_i L_i(x) + \int_a^b \prod_{i=0}^{n}(x - x_i)\frac{f^{(n+1)}(c)}{(n+1)!}dx \quad c \in [a, b] \\ &= \sum_{i=0}^{n} a_i f_i + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x - x_i) f^{(n+1)}(c)dx\end{aligned}$$

Numerical Integration

$a_i = \int_a^b L_i(x)dx$ and therefore $\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f_i$ with error given by

$E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i) f^{(n+1)}(c)dx.$

Following are some of the simplest and best known examples of Newton-Cotes quadrature rules:

- **Mid-point Rule:** One point is given. So, the polynomial is of degree zero i.e. a constant. This point is the midpoint of the interval $x_0 = \frac{a+b}{2}$ and $(\frac{a+b}{2}, f(\frac{a+b}{2}))$ is given.
  $\hat{I}(f) = a_0 f_0 = f_0 \int_a^b 1 \times dx = f_0(b-a) = (b-a)f(\frac{a+b}{2})$. So,

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

and using Taylor expansion not the formula defined above, $E(f) = \int_a^b (x-x_0)f_0' dx + \int_a^b \frac{(x-x_0)^2}{2} f''(c) dx = \frac{1}{24} f''(c)(b-a)^3, c \in [a,b]$

- **Trapezoid Rule:** Two points are given: (x_0, f_0), (x_1, f_1) and polynomial is of degree one.

  $\hat{I}(f) = \sum_{i=0}^{1} a_i f_i$, where $a_0 = \int_a^b L_0(x)dx$ and $a_1 = \int_a^b L_1(x)dx$. By knowing that $x_0 = a$, $x_1 = b$, $a_0 = \frac{b-a}{2}$ and $a_1 = \frac{b-a}{2}$. So,

$$\hat{I}(f) = \frac{1}{2}(b-a)\left[f(a) + f(b)\right]$$

and $E(f) = \int_a^b \frac{f''(c)}{2}(x-x_0)(x-x_1)dx = -\frac{1}{12} f''(c)(b-a)^3$

- **Simpson Rule:** Three equally spaced points are given: (x_0, f_0), (x_1, f_1) and (x_2, f_2) and polynomial is of degree two. $\hat{I}(f) = \sum_{i=0}^{2} a_i f_i$, where $a_0 = \int_a^b L_0(x)dx$, $a_1 = \int_a^b L_1(x)dx$ and $a_2 = \int_a^b L_2(x)dx$. By knowing that $x_0 = a$, $x_1 = a + h$, and $x_2 = b$ and $h = \frac{b-a}{2}$, $a_0 = \frac{b-a}{6}$, $a_1 = \frac{4}{6}(b-a)$ and $a_2 = \frac{b-a}{6}$. So,

$$\hat{I}(f) = \frac{b-a}{6}(b-a)\left[f(a) + 4f(x_1) + f(b)\right]$$

and using Taylor expansion and weighted Mean Value Theorem $E(f) = -\frac{1}{2880} f^{(4)}(c)(b-a)^5$

Examples:

- Compare the Trapezoid and Simpson Rule approximation to calculate $\int_0^2 f(x)dx$ when $f(x) = \sqrt{1+x^2}$

$T(f) = \frac{b-a}{2}(f(0) + f(2)) = 3.326$

$S(f) = \frac{b-a}{6}(f(0) + 4f(1) + f(2)) = 2.964$

Exact=2.958

- The Trapezoidal rule applied to $\int_0^2 f(x)dx$ gives the value 4, and Simpson rule gives the value 2. What is f(1)?
- Approximate the given integral using the Simpson rule: $\int_0^{\frac{\pi}{4}} e^{3x}\sin(2x)dx$
- Approximate the integral $\int_0^{1.5} x^2 ln(x)dx$ using Trapezoidal rule. Give an error band on this approximation.

Measuring Precision: The standard derivation of quadrature error is based on determining the class of polynomial for which these formulas produce exact results.

Definition. The degree of precision of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, $k = 0, \cdots, n$. So, Trapezoidal and Simpson rules have degree of precision one and three respectively. In the other word, the degree of precision of a quadrature formula is n iff the error is zero for all polynomials of degree $k = 0, \cdots, n$, but is not zero for some polynomial of degree $n + 1$.

Examples:

• Find the degree of precision of the quadrature formula

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

• The quadrature formula $\int_0^2 f(x)dx = c_0 f(0) + c_1 f(1) + c_2 f(2)$ is exact for all polynomial of degree less than or equal to 2. Determine c_0, c_1 and c_2.

• Find the constant c_0, c_1 and x_1 so that the quadrature formula $\int_0^1 f(x)dx = c_0 f(0) + c_1 f(1) + c_1 f(x_1)$ has the highest possible degree of precision.

• Use Trapezoidal rule to find $\int_2^{10} f(x)dx$, where f(x) is represented by

x	2	4	6	8	10
f(x)	1	5	8	10	11

Here we have more than two points. To use Trapezoidal formula which we defined for two points, we can divide the whole interval into subintervals containing two points and then apply Trapezoidal rule on each interval: [2,4], [4,6], [6,8] and [8,10].

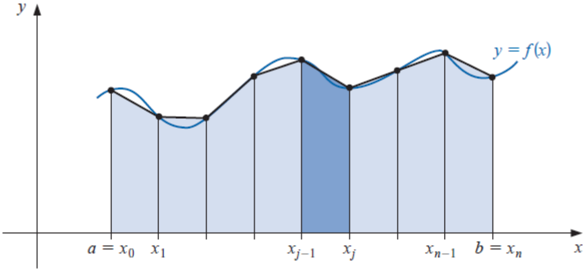
Then, $T(f) = T_1 + T_2 + T_3 + T_4$ in which T_1 is for [2,4], T_2 is for[4,6], T_3 is for [6,8] and T_4 is for[8,10].

$$\begin{aligned} T(f) &= \frac{4-2}{2}(f(2)+f(4)) + \frac{6-4}{2}(f(4)+f(6)) \\ &+ \frac{8-6}{2}(f(6)+f(8)) + \frac{10-8}{2}(f(8)+f(10)) \\ &= 58 \end{aligned}$$

In general if we have n segments, then

$$T(f) = \frac{h}{2}\left(f(a) + \sum_{i=1}^{n-1} 2f(x_i) + f(b)\right), \qquad h = \frac{b-a}{n}$$

This is called **Composite Trapezoidal Rule**.



Composite Trapezoidal Rule(Ref. Numerical Analysis by Burden)

Local truncation error in each segment is $E_i(f) = \frac{h^3}{12} f''(c_i)$ and global truncation error is $E(f) = \sum_{i=1}^{n} E_i(f)$. Therefore,

$$|E(f)| = |\sum_{i=1}^{n} E_i(f)| \leq \sum_{i=1}^{n} |E_i(f)| = \sum_{i=1}^{n} |-\frac{h^3}{12} f''(c_i)| = \frac{h^3}{12} \sum_{i=1}^{n} |f''(c_i)|.$$

If $M = \max |f''(x)|$ for $a \leq x \leq b$, then $|E(f)| \leq \frac{h^3}{12} Mn$. Since $n = \frac{b-a}{h}$, then $|E(f)| \leq \frac{h^2}{12}(b-a)M$.

Example:

- Evaluate the integral $\int_0^4 (1 - e^{-x})dx$ using the composite Trapezoidal rule with $n = 4$.
- Find the number of subintervals required to approximate the given integral to within 10^{-6} using the composite trapezoidal rule $\int_0^{\pi} x \sin(x)dx$
- Determine the values of n and h required to approximate $\int_0^2 e^{2x} \sin(3x)dx$ to within 10^{-4} using composite Trapezoidal rule.

Similarly, we can define **Composite Simpson Rule** as explained in the following example.

Example:

- Use Simpson rule to approximate $\int_0^4 e^x dx$ and compare this

approximation to the case in which four points $(1, e)$, $(2, e^2)$, $(3, e^3)$ and $(4, e^4)$ are used.

Simpson rule: $\int_0^4 e^x dx = \frac{4-0}{6}(f(0) + 4f(2) + f(4)) = 56.77$

Dividing [0,4] into 4 subintervals with length $\frac{1}{2}$ and apply Simpson rule on each subinterval yields:

$$\begin{aligned}\int_0^4 e^x dx &= \int_0^1 e^x dx + \int_1^2 e^x dx + \int_2^3 e^x dx + \int_3^4 e^x dx \\ &= \frac{1}{6}\left(f(0) + 4f(\frac{1}{2}) + f(1)\right) + \frac{1}{6}\left(f(1) + 4f(\frac{3}{2}) + f(2)\right)\end{aligned}$$

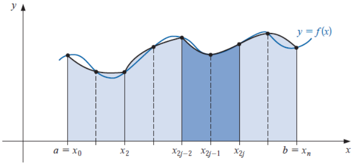
$$+\frac{1}{6}\left(f(2)+4f(\frac{5}{2})+f(3)\right)+\frac{1}{6}\left(f(3)+4f(\frac{7}{2})+f(2)\right)=53.62.$$

Exact answer is 53.60.

In general, **Composite Simpson Rule** is defined as:

$$\int_a^b f(x)dx=\frac{h}{3}\left[f(x_0)+2\sum_{j=1}^{\frac{n}{2}-1}f(x_{2j})+4\sum_{j=1}^{\frac{n}{2}}f(x_{2j-1})+f(x_n)\right]$$

and $E(f)=-\dfrac{b-a}{180}h^4f^{(4)}(c)$.



Composite Simpson Rule(Ref. Numerical Analysis by Burden)

Example:

- Use the composite Trapezoidal and Simpson rule with n=4 to approximate $\int_1^2 x ln(x) dx$
- Evaluate the integral $\int_0^4 xe^{2x} dx$ using composite Simpson rule with $n = 4$.
- Let f(x) be defined as follows. Use the composite Simpson rule with $n = 4$ to approximate $\int_0^2 f(x) dx$.

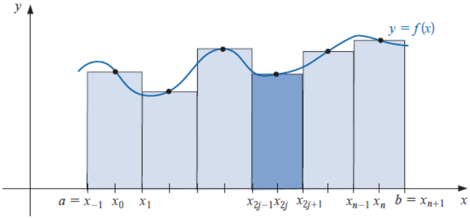
$$f(x) = \begin{cases} x + 3 & 0 \leq x \leq 1 \\ 4 + 2(x-1)^2 & 1 \leq x \leq 2 \end{cases}$$

Numerical Integration

In the same way, **Composite Mid-point Rule** for n+2 subinterval can be written as

$$\int_a^b f(x)dx = 2h\sum_{j=0}^{\frac{n}{2}} f(x_{2j})$$

and $E(f) = \dfrac{b-a}{6}h^2 f''(c)$.

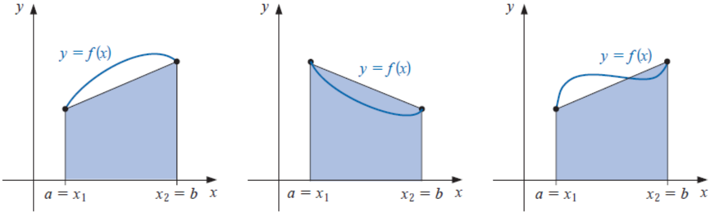


Composite Mid-Point Rule(Ref. Numerical Analysis by Burden)

Example:

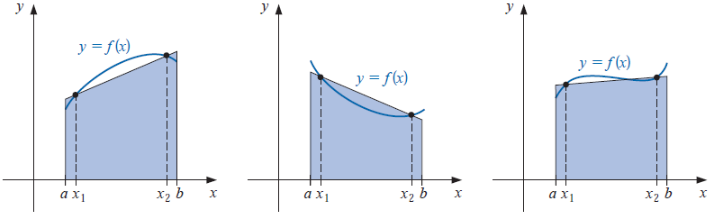
• Evaluate the integral $\int_0^1 \frac{1}{x+4}dx$ using the composite mid-point rule with $n = 6$.

Gaussian Quadrature:
The Newton-Cotes formulas were derived by integrating interpolating polynomials. The error term in the interpolating polynomial of degree n involves the (n+1)th derivative of the function being approximated. So, a Newton-Cotes formula is exact when approximating the integral of any polynomial of degree less than or equal to n.
All the Newton-Cotes formulas use values of the function at equally-spaced points. This restriction is convenient when the formulas are combined to form the composite rules, but it can decrease the accuracy of the approximation. For example, if we use Trapezoidal rule to determine the integral of the functions whose graphs are shown



Ref. Numerical Analysis by Burden

The Trapezoidal rule approximates the integral of f(x) by integrating the linear function that joins the endpoints of the graph of the function. This is not likely the best line for approximating the integral. For example the following line can give much better approximation in most cases



Ref. Numerical Analysis by Burden

Gaussian Quadrature chooses the points for evaluation in an optimal, rather than equally spaced way. The nodes $x_1, x_2, \cdots, x_n$ in [a,b] and coefficients $w_1, \cdots, w_n$ are chosen to minimize the expected error obtained in the approximation $\displaystyle\int_a^b f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i)$.

To measure this accuracy, we assume that the best choice of these values produces the exact result for the largest class of polynomials, that is, the choice that gives the greatest degree of precision.
The coefficients $w_1, \cdots, w_n$ in the approximation formula are arbitrary, and the nodes $x_1, x_2, \cdots, x_n$ are restricted only by the fact that they must lie in [a, b], the interval of integration. This gives us 2n parameters to choose. If the coefficients of a polynomial are considered parameters, the class of polynomials of degree at most 2n-1 also contains 2n parameters. This is then the largest degree of polynomials for which integral is exact.
For illustration, we assume $n = 2$ and the interval of integration is [-1,1].
Then, $\displaystyle\int_{-1}^{1} f(x)dx = w_1 f(x_1) + w_2 f(x_2)$. This integral is exact for f(x) as a polynomial of degree 3 $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$ for some values of a_0, a_1, a_2 and a_3. Integral is exact when $f(x)$ is $1, x, x^2$ and x^3 because

$$\int f(x)dx = a_0 \int 1dx + a_1 \int xdx + a_2 \int x^2 dx + a_3 \int x^3 dx.$$

$$\int_{-1}^{1} 1dx = w_1 + w_2 = 2 \qquad \int_{-1}^{1} xdx = w_1x_1 + w_2x_2 = 0$$

$$\int_{-1}^{1} x^2dx = w_1x_1^2 + w_2x_2^2 = \frac{2}{3} \qquad \int_{-1}^{1} x^3dx = w_1x_1^3 + w_2x_2^3 = 0$$

Solving these equations gives $w_1 = w_2 = 1$ and $x_1 = -\frac{\sqrt{3}}{3}$ and $x_2 = \frac{\sqrt{3}}{3}$.

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

This formula has degree of precision 3 and produces the exact results for every polynomial of degree 3 or less.

Proposition: Gaussian Integration

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

is an approximation for $I = \int_a^b f(x)dx$ with degree of precision 3.

Example:

- Find $\int_1^3 \left[x^6 - x^2 sin(2x)\right] dx$ using Gaussian integration.

$\hat{I} = \frac{3-1}{2}\left[f\left((\frac{3-1}{2})(-\frac{1}{\sqrt{3}}) + \frac{3+1}{2}\right) + f\left((\frac{3-1}{2})(\frac{1}{\sqrt{3}}) + \frac{3+1}{2}\right)\right] \approx$ 302.4

Exact=317.3

- Evaluate $\int_0^{\frac{\pi}{4}} cos^2(x)dx$ using Gaussian integration.

Exact=0.6427