MATH 5520
Numerical Integration 1.

Dmitriy Leykekhman

Spring 2009

Numerical Integration.

- Our goal is to compute
$$\int_a^b f(x)\, dx.$$
- Even if $f(x)$ can be expressed in terms of elementary functions, the antiderivative of $f(x)$ may not have this property. For example: e^{-x^2}, $\sin(x^2)$, $\frac{\sin x}{x}$, etc.
- All exact techniques of integration taught in Calculus courses are more like exceptions then the rules.
- As a general rule on must rely on numerical integration.

Numerical Integration.

- We want to approximate the integral of a function f by a weighted sum of function values:

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

- In the above formula $x_i \in [a, b]$ are called the nodes of the integration formula and w_i are called the weights of the integration formula.
- When we approximate $\int_a^b f(x)\,dx$ by $\sum_{i=0}^{n} w_i f(x_i)$ we speak of numerical integration or numerical quadrature
- $\sum_{i=0}^{n} w_i f(x_i)$ is called a quadrature formula.

Numerical Integration.

Introduce a new variable

$$x = a + \frac{b-a}{\beta-\alpha}(z-\alpha)$$

. Then if $z = \alpha$, $x = a$ and if $z = \beta$, $x = b$, furthermore

$$dx = \frac{b-a}{\beta-\alpha}dz$$

and by the change of variable formula

$$\int_a^b f(x)\ dx = \frac{b-a}{\beta-\alpha}\int_\alpha^\beta f\left(a + \frac{b-a}{\beta-\alpha}(z-\alpha)\right)\ dz.$$

Numerical Integration.

Thus, if we have computed weights $\widehat{w}_i$ and nodes $\widehat{z}_i$ for the numerical integration on an interval $[\alpha, \beta]$, then we can use the above identity to approximate the integral of f over any interval $[a, b]$ (assuming, of course, that this integral exist) by

$$\int_a^b f(x)\, dx = \frac{b-a}{\beta-\alpha} \int_\alpha^\beta f\left(a + \frac{b-a}{\beta-\alpha}(z-\alpha)\right)\, dz$$
$$\approx \frac{b-a}{\beta-\alpha} \sum_{i=0}^{n} \widehat{w}_i f\left(a + \frac{b-a}{\beta-\alpha}(\widehat{z}_i-\alpha)\right).$$

Numerical Integration.

That is, the weights w_i and nodes x_i for the numerical integration on the interval $[a, b]$ are

$$w_i = \frac{b-a}{\beta-\alpha}\widehat{w}_i, \quad x_i = a + \frac{b-a}{\beta-\alpha}(\widehat{z}_i - \alpha).$$

This means it is sufficient to compute weights and nodes for the numerical integration on a certain interval like $[0, 1]$ or $[-1, 1]$, often called the reference intervals.

Numerical Integration.

Before we discuss several quadrature methods, we summarize some properties of the integral which are important for the development of quadrature rules. First, we note that

$$\int_a^b 1 \, dx = b - a.$$

Therefore we require

$$\sum_{i=0}^{n} w_i = b - a,$$

Otherwise, our quadrature formula could not even evaluate the integral of a constant function exactly.

Numerical Integration.

Another property of the integral is

$$f(x) \geq 0 \quad \Longrightarrow \int_a^b f(x)\, dx \geq 0.$$

If

$$w_i \geq 0, \quad i = 0, \ldots, n,$$

then

$$\sum_{i=0}^{n} w_i f(x_i) \geq 0,$$

for all functions $f(x) \geq 0$.

Numerical Integration.

- We also desire our numerical quadrature to be efficient.
- Efficiency often depends upon the number of function evaluations.
- Typically to evaluate f at x_i is more expensive than form a linear combination of function values.

Interpolatory Quadrature Formulas.

Basic idea: if $p(x)$ is some function such that

$$p(x) \approx f(x),$$

then

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

Thus we need a function $p(x)$ which close to $f(x)$ and easy to integrate.

Interpolatory Quadrature Formulas.

Chose nodes $x_0, x_1, \dots, x_n$ in the interval $[a, b]$ and compute the polynomial $P(f|x_0, \dots, x_n)$ of degree less or equal to n interpolating f at $x_0, x_1, \dots, x_n$. If we use the approximation

$$f(x) \approx P(f|x_0, \dots, x_n)(x),$$

then we obtain an approximation for the integral:

$$\int_a^b f(x)\, dx \approx \int_a^b P(f|x_0, \dots, x_n)(x)\, dx \quad (1). \tag{1}$$

These types of quadrature formulas are called interpolatory quadrature formulas.

Interpolatory Quadrature Formulas.

It is useful to represent the interpolation polynomial using the Lagrange basis,

$$P(f|x_0,\dots,x_n)(x) = \sum_{i=0}^{n} f(x_i) \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}.$$

If we substitute this representation of the interpolation polynomial into (1), then we obtain

$$\begin{aligned}
\int_a^b f(x)\,dx &\approx \int_a^b P(f|x_0,\dots,x_n)(x)\,dx \\
&= \int_a^b \sum_{i=0}^{n} f(x_i) \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx \\
&= \sum_{i=0}^{n} f(x_i) \int_a^b \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx.
\end{aligned}$$

Interpolatory Quadrature Formulas.

This leads to the quadrature formula

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

where

$$wi = \int_a^b \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx.$$

Midpoint Rule.

The simplest quadrature formula can be constructed using $n = 0$ and $x_0 = \frac{a+b}{2}$. Since

$$\prod_{\substack{j=0 \\ j \neq i}}^{0} \frac{x - x_j}{x_i - x_j} = 1$$

we obtain the **midpoint rule:**

$$\int_a^b f(x)\, dx \approx (b-a) f\left(\frac{a+b}{2}\right).$$

Trapezoidal Rule.

The next quadrature formula is constructed using $n = 1$ and $x_0 = a$, $x_1 = b$. It holds that

$$\int_a^b \frac{x-a}{b-a} dx = \frac{b-a}{2}, \quad \int_a^b \frac{x-b}{a-b} dx = \frac{b-a}{2}.$$

This yields the **Trapezoidal rule**:

$$\int_a^b f(x)\ dx \approx \frac{b-a}{2}(f(a)+f(b)).$$

Simpson rule.

The next quadrature formula is constructed using $n = 2$ and $x_0 = a$, $x_1 = \frac{b+a}{2}$, $x_2 = b$. Then

$$\int_a^b \frac{x - \frac{b+a}{2}}{a - \frac{b+a}{2}} \frac{x-b}{a-b} dx = \frac{b-a}{6},$$

$$\int_a^b \frac{x-a}{\frac{b+a}{2} - a} \frac{x-b}{\frac{b+a}{2} - b} dx = 4\frac{b-a}{6},$$

$$\int_a^b \frac{x - \frac{b+a}{2}}{b - \frac{b+a}{2}} \frac{x-b}{b-a} dx = \frac{b-a}{6}.$$

This yields the **Simpson rule**:

$$\int_a^b f(x)\, dx \approx \frac{b-a}{6}\left(f(a) + 4f\big(\frac{b+a}{2}\big) + f(b)\right).$$

Newton Cotes Quadrature Formula.

If we have equidistant points

$$x_i = a + ih, \quad i = 0, \dots, n, \quad h = \frac{b-a}{n},$$

then the resulting interpolatory quadrature formula is called a **closed Newton Cotes quadrature formula** (a and b are nodes). In this case we can use the substitution $x = a + sh$, to compute

$$w_i = \int_a^b \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} dx = (b-a)\frac{1}{n}\int_0^n \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{s-j}{i-j}\, ds.$$

Newton Cotes Quadrature Formula.

If we have equidistant points

$$x_i = x_0 + ih, \quad i = 0, \dots, n,$$

where

$$h = \frac{b-a}{n+2}, \quad x_0 = a + h, \quad x_n = b - h,$$

then the resulting interpolatory quadrature formula is called an **open Newton Cotes quadrature formula** (a and b are not nodes). Again, we can use the substitution $x = a + sh$, to compute

$$w_i = \int_a^b \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} dx = (b-a)\frac{1}{n+2}\int_0^n \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{s-j}{i-j}\, ds.$$

Newton Cotes Quadrature Formula.

Since the interpolation polynomial is uniquely determined, the interpolating polynomial for a polynomial p_n of degree less or equal to n is the polynomial itself:

$$P(p_n|x_0,\ldots,x_n)(x) = p_n(x).$$

This implies that

$$\int_a^b p_n(x)dx = \int_a^b P(p_n|x_0,\ldots,x_n)(x)dx = \sum_{i=1}^n w_i p_n(x_i)$$

for all polynomials p_n of degree less or equal to n. If

$$\int_a^b p_n(x)dx = \sum_{i=0}^n w_i p_n(x_i)$$

for all polynomials p_n of degree less or equal to n we say that the integration method is exact of degree n.

Newton Cotes Quadrature Formula.

One can even show the following result.

Theorem (Exactness of Newton Cotes Formulas)

Let $a \leq x_0 < \cdots < x_n \leq b$ be given and let w_i be the nodes and weights of a Newton Cotes formula. If n is even, then the quadrature formula is exact for polynomials of degree $n+1$. If n is odd, then the quadrature formula is exact for polynomials of degree n.

Table of Newton Cotes Quadrature Formulas.

The weights and nodes for the most popular NewtonCotes formulas are summarized in the table below.

$n+1$	$\widehat{w}_i$	error	name
2	$\frac{1}{2}, \frac{1}{2}$	$h^3 \frac{1}{12} f^{(2)}(\xi)$	Trapezoidal rule
3	$\frac{1}{6}, \frac{4}{6}, \frac{1}{6}$	$h^5 \frac{1}{90} f^{(4)}(\xi)$	Simpsons rule
4	$\frac{1}{8}, \frac{3}{8}, \frac{3}{8}, \frac{1}{8}$	$h^5 \frac{3}{80} f^{(4)}(\xi)$	3/8rule
5	$\frac{7}{90}, \frac{32}{90}, \frac{12}{90}, \frac{32}{90}, \frac{7}{90}$	$h^7 \frac{8}{945} f^{(6)}(\xi)$	Milnes rule

In the table

$$w_i = \widehat{w}_i(b-a), \quad x_i = a + ih, \quad i = 0, \dots, n, \quad h = \frac{b-a}{n}.$$