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Mechanical Quadrature Methods from Fitting Least Squire Interpolation Polynomials

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Abstract: In this paper, we are developing Quadrature Methods (*numerical integration method*) of continuous function $f(x)$ on a compact interval $[a, b]$ and deriving a polynomial $P_m(x)$ of degree m such that integration of $P_m(x)$ from a to b is equal to integration of $f(x)$ from a to b. We are using least square method to fit the polynomial $P_m(x)$. Also derive Newton-Cotes formulas and composite formula from this method, estimate errors and given MATLAB codes.

Key Words: Numerical integration, Newton-cotes method, quadrature method.

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§1. Introduction

With the advent of the modern high speed electronic digital computers, the Numerical Integration have been successfully applied to study problems in Mathematics, Engineering, Computer Science and Physical Sciences. Numerical integration, also called *Quadrature*, is the study of how the numerical value of an integral can be found. The purpose of this paper is quadrature methods for approximate calculation of definite integrals

$$I[f] = \int_a^b f(x)dx \tag{1.1}$$

where $f(x)$ is integrable, in the Riemann sense on $[a, b]$. The limit of the integration may be finite. Numerical integration is always carried out by mechanical quadrature and its basic scheme is as follows:

$$\int_a^b f(x) = \sum_{i=0}^{n-1} A_i f_i + R[f], \tag{1.2}$$

where $f_i = f(x_i)$ is continuous function in$[a, b]$. $A_i$and x_i are called *Coefficients(Weights)* and *nodes* for Numerical Quadrature, respectively, and R[f] is error of Quadrature method. Once the coefficients and nodes are set down, the scheme (1) can be determined.

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§2. Preliminaries

2.1 Order of Quadrature Method

Order of accuracy, or precision, of a Quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \cdots, n$.

2.2 Error of Quadrature Method

The integration (1.1) is approximated by a finite linear combination of value of $f(x)$ in the form (1.2). The error of approximation of (1.2) is given as

$$R_n = \frac{C}{(m+1)!} f^{(m+1)}(\xi), \tag{2.1}$$

where $\xi = (a, b)$, $m \geq n$ is order of (1.2) and error constant of (1.2) is

$$C = \int_a^b x^{m+1} - \sum_{i=0}^{n-1} A_i x_i^{m+1}. \tag{2.2}$$

2.3 Interpolation Polynomial

Let $f(x)$ be a continuous function defined on some interval $[a, b]$, and be prescribed at $n+1$ distinct tabular points $x_0, x_1, \cdots, x_n$ such that $a = x_0 < x_1 < x_2 < \cdots < x_n = b$. The distinct tabular points $x_0, x_1, \cdots, x_n$ are equispaced, that is $x_{k+1} - x_k = h$, $k = 0, 1, 2, \cdots, n-1$. The problem of polynomial approximation is to find a polynomial $P_n(x)$, of degree$\leq n$, which fits the given data exactly, that is,

$$P_n(x_i) = f(x_i), i = 0, 1, 2, \cdots, n. \tag{2.3}$$

The polynomial $P_n(x)$ is called the interpolating polynomial. The conditions given in (5)are called the interpolating conditions.

2.4 Least Squares Interpolation Polynomial

Let the polynomial of the m^{th} degree

$$P_m(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m$$

be fitted to the data points $(x_i, f(x_i))$ $i = 0, 1, 2, \cdots, n$, where $m < n$ and $a_i's$ are satisfy the the system of equations

$$(n+1)a_0 + a_1 \sum_{i=0}^{n} x_i + a_2 \sum_{i=0}^{n} x_i^2 + \cdots + a_m \sum_{i=0}^{n} x_i^m = \sum_{i=0}^{n} f(x_i), \tag{2.4}$$

$$a_0\sum_{i=0}^{n} x_i + a_1\sum_{i=0}^{n} x_i^2 + \cdots + a_m\sum_{i=0}^{n} x_i^{m+1} = \sum_{i=0}^{n} x_i f(x_i)$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$a_0\sum_{i=0}^{n} x_i^m + a_1\sum_{i=0}^{n} x_i^{m+1} + \cdots + a_m\sum_{i=0}^{n} x_i^{2m} = \sum_{i=0}^{n} x_i^m f(x_i).$$

There are $m+1$ equations in $m+1$ unknowns.

Lemma 2.1 *Let $P_m(x)$ be the least squares interpolation equation of $f(x)$ on $[a,b]$. Then*

$$\sum_{i=0}^{n} P_m(x_i) \approx \sum_{i=0}^{n} f(x_i), \tag{2.5}$$

where $x_0 = a, x_n = b$, $x_i = a + ih$ and $h = (b-a)/n$.

Proof Let the $P_m(x) = a_0 + a_1x + a_2x^2 + \cdots + a_mx^m$ is least squares interpolation equation of $f(x)$ on $[a,b]$. Then $P_m(x_0) = a_0 + a_1x_0 + a_2x_0^2 + \cdots + a_mx_0^m$ and $P_m(x_1) = a_0 + a_1x_1 + a_2x_1^2 + \cdots + a_mx_1^m$, and so on $P_m(x_n) = a_0 + a_1x_n + a_2x_n^2 + \cdots + a_mx_n^m$. Adding all we get

$$\sum_{i=0}^{n} P_m(x_i) = (n+1)a_0 + a_1\sum_{i=0}^{n} x_i + a_2\sum_{i=0}^{n} x_i^2 + \cdots + a_m\sum_{i=0}^{n} x_i^m$$

apply Equation (2.4), we get

$$\sum_{i=0}^{n} P_m(x_i) \approx \sum_{i=0}^{n} f(x_i).$$

□

Theorem 2.2 *Let $P_m(x)$ is least squares interpolation equation of the integrable function $f(x)$ on finite interval $[a,b]$ and*

$$\sum_{i=0}^{n} P_m(x_i) \cong \sum_{i=0}^{n} f(x_i),$$

where $x_0 = a, x_n = b$ if and only if

$$\int_{x_0}^{x_n} P_m(x)dx \cong \int_{x_0}^{x_n} f(x)dx. \tag{2.6}$$

Proof Multiplying with $h = (b-a)/n$ and take limit $h \longrightarrow 0$ in (2.5), we get

$$\lim_{h\longrightarrow 0} h\sum_{n=0}^{n} P_m(x_n) = \lim_{h\longrightarrow 0} h\sum_{n=0}^{n} f(x_n).$$

This completes the theorem. □

§3. Least Square Quadrature Method

Consider the integral in the form (1.2) for each $i = 0, 1, 2, \cdots, n$. Now we are dividing the interval $[a, b]$ into n (finite) equal sub interval and take the nodes $x's$ are equispaced points such that $x_i = x_0 + ih \in [a, b]$, $i = 0, 1, 2, \cdots, n$, where $x_0 = a, x_n = b$ and $h = (b-a)/(n)$. So we have data points $(x_i, f(x_i))$ $i = 0, 1, 2, \cdots, n$ for fit a polynomial $P_m(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m$. we have

$$\begin{aligned}\int_{x_0}^{x_n} f(x)dx &= \int_{x_0}^{x_n} P_m(x)dx \\ &= a_0(x_n - x_0) + a_1 \frac{x_n^2 - x_0^2}{2} + a_2 \frac{x_n^3 - x_0^3}{3} + \cdots + a_m \frac{x_n^{m+1} - x_0^{m+1}}{m+1}. \qquad (3.1)\end{aligned}$$

This method is called L_m^n -Quadrature method($L_m^n - rule$), here m is donate degree of polynomial and n is donate number of data points. To solve the least square Quadrature method we have at least m+1 points. Order of this method is greater then or equal to m, since it's exact for polynomial of degree m. The error constant of (3.1) is

$$C = \int_{x_0}^{x_n} x^k - a_0 + \sum_{i=1}^{n} \frac{x_n^i - x_0^i}{i} a_i$$

and error

$$R = \frac{C}{k!} f^{(k)}(\xi),$$

where $k \geqslant m, a \leqslant \xi \leqslant b$. Now following cases arise:

Case 1. $m = 0$, that is P_0 is a constant function.

From (2.4) we have $a_0(n+1) = \sum_{i=0}^{n} f(x_i)$ and $a_1 = a_2 = \cdots = a_m = 0$, substituting this values in (9) web get

$$\int_{x_0}^{x_n} f(x)dx = \frac{(x_n - x_0)}{n+1} \sum_{i=1}^{n} f(x_i). \qquad (3.2)$$

Case 2. $m = 1$, that is P_1 is a linear polynomial.

From (2.4) we have

$$a_0(n+1) + a_1 \sum_{i=0}^{n} x_i = \sum_{i=0}^{n} f_i, a_0 \sum_{i=0}^{n} x_i + a_1 \sum_{i=0}^{n} x_i^2 = \sum_{i=0}^{n} x_i f_i$$

and $a_2 = a_3 = \cdots = a_m = 0$. Solving for a_1 and a_2 we get

$$a_0 = \frac{\sum_{i=0}^{n} f_i \sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i \sum_{i=0}^{n} x_i f_i}{(n+1)\sum_{i=0}^{n} x_i^2 - (\sum_{i=0}^{n} x_i)^2},$$

$$a_1 = \frac{(n+1)\sum_{i=0}^{n} x_i f_i - \sum_{i=0}^{n} x_i \sum_{i=0}^{n} f_i}{(n+1)\sum_{i=0}^{n} x_i^2 - (\sum_{i=0}^{n} x_i)^2}.$$

After simplification we get

$$a_0 = \frac{2}{nh(n+1)(n+2)} \left[n(3x_0 + h(n+1)) \sum_{i=0}^{n} f_i - 3(x_0 + x_n) \sum_{i=0}^{n} i f_i \right],$$

$$a_1 = \frac{6}{nh(n+1)(n+2)}\left[2\sum_{i=0}^{n} if_i - i\sum_{i=0}^{n} f_i\right].$$

Substituting this values in (3.1), and simplification we get

$$\int_{x_0}^{x_n} f(x)dx = \frac{nh}{n+1}\sum_{i=1}^{n} f(x_i).$$

This is same as $m = 0$. The method (3.2) is called L_1^n- Quadrature method and the error constant of (3.2) is

$$C = \int_{x_0}^{x_n} x^2dx - \frac{nh}{n+1}\sum_{i=0}^{n}(x+ih)^2 = \frac{-h^3n^2}{6} = \frac{-(x_n-x_a)^3}{6n} = -\frac{(b-a)^3}{6n}$$

and error of (3.2) is

$$R = \frac{-(b-a)^3}{6n\cdot 2!}f^{(2)}(\xi) = \frac{-(b-a)^3}{12n}f^{(2)}(\xi), \tag{3.3}$$

where $x_0 \leqslant \xi \leqslant x_n$. To solve this method, we have at least 2 data points and the order of (3.2) is 2.

Case 3. $m = 2$, that is P_2 is a polynomial of degree two.

From (2.4) we have

$$(n+1)a_0 + a_1\sum_{i=0}^{n} x_i + a_2\sum_{i=0}^{n} x_i^2 = \sum_{i=0}^{n} f_i = A,$$

$$a_0\sum_{i=0}^{n} x_i + a_1\sum_{i=0}^{n} x_i^2 + a_2\sum_{i=0}^{n} x_i^3 = \sum_{i=0}^{n}(x_0+ih)f_i = Ax_0 + hB,$$

$$a_0\sum_{i=0}^{n} x_i^2 + a_1\sum_{i=0}^{n} x_i^3 + a_2\sum_{i=0}^{n} x_i^4 = \sum_{i=0}^{n}(x_0+ih)^2f_i = Ax_0^2 + 2Bhx_0 + Ch^2,$$

where $A = \sum_{i=0}^{n} f_i$, $B = \sum_{i=0}^{n} if_i$, and $C = \sum_{i=0}^{n} i^2f_i$. we have $a_3 = a_4 = \cdots = a_m = 0$.

Solving the three linear system of equation for a_0, a_1 and a_2 by MATLAB, we get

$$\begin{aligned} a_0 \;=\; & \frac{3}{(n+1)(n^3+4n^2+n-6)h^2n} \\ & \times(3Ah^2n^4 + 12Ahn^3x_0 - 12Bh^2n^3 - Ah^2n^2 - 6Ahn^2x_0 + 10An^2x_0^2 \\ & +6Bh^2n^2 - 64Bhn^2x_0 + 10Ch^2n^2 - 2Ah^2n - 6Ahnx_0 - 10Anx_0^2 \\ & +6Bh^2n - 8Bhnx_0 - 60Bnx_0^2 - 10Ch^2n + 60Chnx_0 + 12Bhx_0 + 60Cx_0^2) \end{aligned}$$

$$\begin{aligned} a_1 \;=\; & -\{6(6Ahn^3 - 3Ahn^2 + 10An^2x - 32Bhn^2 - 3Ahn - 10Anx \\ & -4Bhn - 60Bnx + 30Chn + 6Bh + 60Cx)\}/h^2n(n^2+3n+2)(n^2+2n-3) \end{aligned}$$

and

$$a_2 = \frac{30(An^2 - An - 6Bn + 6C)}{h^2 n(n^4 + 5n^3 + 5n^2 - 5n - 6)}.$$

Substituting these values in (3.1), and simplification we get

$$\int_{x_0}^{x_n} f(x)dx = \frac{hn(An^3 - An^2 + 6An + 30Bn - 6A - 30C)}{(n-1)(n+3)(n+2)(n+1)}.$$

Substituting A, B and C we get

$$\int_{x_0}^{x_n} f(x)dx = \frac{hn}{(n-1)(n+3)(n+2)(n+1)} \sum_{i=0}^{n} (n^3 - n^2 + 6n - 6 + 30ni - 30i^2) f_i. \tag{3.4}$$

This method is called L_2^n-Quadrature method. To solve this method, we have at least 3 data points.

Case 4. $m = 3$, that is P_3 is a polynomial of degree three.

Following previous case we get the same as (3.3). The error constant of (3.4) is

$$\begin{aligned} C &= \int_{x_0}^{x_n} x^4 dx - \frac{hn}{(n-1)(n+3)(n+2)(n+1)} \sum_{i=0}^{n} (n^3 - n^2 + 6n - 6 + 30ni - 30i^2)(x + ih)^4 \\ &= -\frac{(3n^2 - 8n + 18)n^2 h^5}{210} = -\frac{(3n^2 - 8n + 18)(x_n - x_0)^5}{210n^3} = -\frac{(3n^2 - 8n + 18)(b-a)^5}{210n^3}. \end{aligned}$$

The error of (3.4) is

$$R = -\frac{(3n^2 - 8n + 18)(b-a)^5}{210n^3 \cdot 4!} f^{(4)}(\xi), \tag{3.5}$$

where $a \leqslant \xi \leqslant b$. The order of (3.4) is 4.

Note 3.1 If $m \geqslant 0$ is even number then L_m^n method same as L_{m+1}^n method.

§4. Newton-Cotes Formulas from Least Square Method

We can derive trapezoidal rule, Simpson 1-3rd rule and Simpson 3-8th rule from least square method.

Taking $n = 1$ in (3.2) we get

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1).$$

This formula is called trapezoidal rule. The error of trapezoidal rule is, from (3.3)

$$R = \frac{-(b-a)^3}{12} f^{(2)}(\xi), \quad a \leqslant \xi \leqslant b.$$

Taking $n = 2$ in (3.4) we get

$$\int_{x_0}^{x_2} f(x)dx = \frac{2h}{1 \cdot 5 \cdot 4 \cdot 3} \sum_{i=0}^{2} (10 + 60i - 30i^2) f_i$$
$$= \frac{h}{30}(10f_0 + 40f_1 + 10f_2) = \frac{h}{3}(f_0 + 4f_1 + f_2).$$

This formula is called Simpson 1-3rd rile rule. The error Simpson 1-3rd rule of is, from (3.5)

$$R = \frac{-(b-a)^5}{90} f^{(4)}(\xi), a \leqslant \xi \leqslant b.$$

Similarly, Simpson 3-8th rule come from (3.4) with $n = 3$, that is

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

and error come from (3.5), $R = -(3/80)h^5 f^{(4)}(\xi), a \leqslant \xi \leqslant b$.

The weights of the integration method of (3.4) with equispaced point for $n \leq 6$ are given in Table 1.

n	comman ratio	Newton-Cotes weight	common ratio	L_2^n Method
1	1/2	1 1	—	—
2	1/3	1 4 1	1/3	1 4 1
3	3/8	1 3 3 1	3/8	1 3 3 1
4	2/45	7 32 12 32 7	4/105	11 26 31 26 11
5	5/288	19 75 50 50 75 19	5/336	31 61 78 78 61 31
6	1/140	41 216 27 272 27 216 41	1/14	7 12 15 16 15 12 7

Table 1. Weight of Newton-cote rules and Weights of L_2^n Quadrature Method

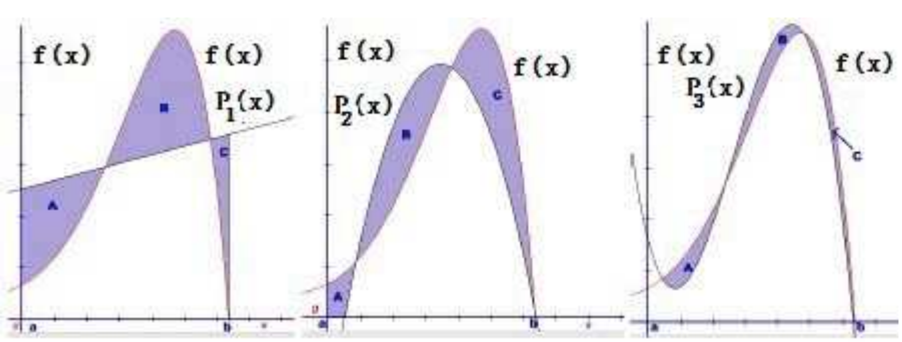

Figure 1 a, b, c

§5. Graphically Meaning of Least Square Integration Method

Let the polynomial $P_m(x)$ of degree m is fitted by least square interpolation method by using data points (x_i, f_i) $i = 0, 1, 2 \cdots, n,$. If m=1, take n is large number then the the polynomial $P_1(x)$ is going to exact fit polynomial such that the area A+C=B $(fib : 1(a))$. That's way the integration of $P_1(x)$ on $[a, b]$ is gives exact value of integration of $f(x)$ on $[a, b]$. Similarly $P_2(x)$ (or $P_3(x)$) is best interpolation polynomial such that the area A+C=B, such as those shown in Figure 1.

§6. Problems

Problem 6.1 Find approximate value of

$$I = \int_1^3 sin(x)e^x dx$$

fit a straight line $y(x)$ such that $\int_1^3 y(x)dx = I$.

Solution Let $f(x) = sin(x)e^x$ and y_n be the straight line by fit n+1 data points $(x_i, f(x_i))$, $i = 0, 1, 2, \cdots, n$. Now we divide the interval [1 3] into two equal subinterval, that is $n = 2$ or $h = 1$. then 3 data points are $(1, f(1))$, $(2, f(2))$ and $(3, f(3))$. we fit a straight line y_2 by normal equation (5) we get

$$y_2 = 0.27x + 3.4$$

following this we get

$$y_4 = 0.78x + 3.15,$$

$$y_8 = 1.17x + 2.77$$

$$y_{16} = 1.39x + 2.51$$

$$y_{32} = 1.51x + 2.36$$

and

$$y_{64} = 1.57x + 2.28.$$

But we know if $n \to \infty$ then $\int_1^3 y_n(x)dx \to \int_1^3 f(x)dx$. Therefore, $I = \int_1^3 (1.57x + 2.28)dx = 10.84$.

Problem 6.2 Fit quadratic equation $P_2(x)$ such that

$$\int_0^1 P_2(x)dx = \int_0^1 x\sqrt{x+1}dx$$

and find approximate value of $\int_0^1 x\sqrt{x+1}dx$.

Solution Let P_{2_n} be the quadratic equation by fit n equal space data points in [0, 1]. By least square method we have

$$\begin{aligned} P_{2_3}(x) &= 0.37893738x^2 + 1.03527618x + 3.61400724(E-20), \\ P_{2_{11}}(x) &= 0.37892845x^2 + 1.03956285x - 0.00227848, \\ P_{2_{51}}(x) &= 0.37839273x^2 + 1.04141576x - 0.00304322, \\ P_{2_{101}}(x) &= 0.3783134x^2 + 1.0416701x - 0.00314653. \end{aligned}$$

Let $I_n = \int_0^1 P_{2_n}(x)dx$ then $I_3 = 0.643950551$, $I_{11} = 0.643812428$, $I_{51} = 0.643795564$ and $I_{101} = 0.643792992$. The exact value of $\int_0^1 x\sqrt{x+1}dx$ upto five decimal is 0.64379.

Problem 6.3 Find the approximate value of

$$I = \int_0^1 \frac{1}{2+x} dx,$$

using L_1^n and L_2^n rules with different equal subintervals. Using the exact solution, find the absolute errors.

Solution Results for the L_1^n and L_2^n rules to estimate the integral of $f(x) = 1/(2+x)$ from x = 0 to 1. The exact value is $I_{exact} = \int_0^1 1/(2+x)dx = ln(x+2)]_0^1 = ln(3) - ln(2)$=0.4054651. We get

n	$I_1^n = L_1^n$ method	Error=$I_1^n - I_{exact}$
1	0.4167	0.0112
2	0.4111	0.0056
4	0.4083	0.0028
8	0.4069	0.0014
16	0.4062	0.0007
32	0.4058	0.0003
64	0.4056	0.0001

n	$I_2^n = L_2^n$ method	Error=$I_2^n - I_{exact}$
2	0.4055556	0.0000905
4	0.4054930	0.0000279
8	0.4054801	0.0000150
16	0.4054735	0.0000084
32	0.4054696	0.0000045
64	0.4054675	0.0000024
128	0.4054663	0.0000012

§7. Conclusion

We develop this new method for easy to solve Definite Integral of finite interval with equispaced nodes and derived Simpson 1/3rd rule and Simpson 3/8th rule from L_2^n Quadrature Method. In this method (L_2^n) weights are increasing from a to midpoint(i.e $(a+b)/2$) of interval and decreasing from midpoint to b. The advances is the weights of $L_2^n - method$ are positive (since($n^3 - n^2 + 6n - 6 + 30ni - 30i^2) \geq 0$ for all $n \geq 2$ for all i) . We have given the MATLAB code also, give any continuous function $f(x)$ on $[a, b]$ that will be give an approximation integration value of $f(x)$ from a to b. Also, we are developing this concept to high degree polynomials and high dimension.

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