NUMERICAL DIFFERENTIATION AND INTEGRATION

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Lecture series on “ Numerical Techniques and Programming in MATLAB”

VBS Purvanchal University, Jaunpur

July 22-28, 2016

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Numerical Differentiation

Basic problems

- Derive a formula that approximates the derivative of a function in terms of linear combination of function values (Function may be known)

- Approximate the value of a derivative of a function defined by discrete data.

Solution Approaches ..

- Use Taylor Series Expansion.
- Pass a polynomial through the given data and differentiate the interpolating polynomial.

Applications

To solve Ordinary and Partial Differential Equations.

First Derivative..

Let $f : [a, b] \longrightarrow \mathbb{R}$, then the derivative of f is another function say $f^{'} : [a, b] \longrightarrow \mathbb{R}$ and defined by

$$f'(c) = \lim_{h \to 0} \frac{f(c+h) - f(c)}{h}, \qquad \forall c \in (a, b).$$

Geometrically Speaking $f'(c)$ is the slope of tangent to the curve $f(x)$ at $x = c$.

Taylor Series

Derivative of a function at $x = x_0$

Suppose f has two continuous derivatives. Then, by Taylor's Theorem

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(\theta)$$

where $\theta \in (x_0, x_0 + h)$. Now,

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

Called Forward Formula

Error

$Error = |\text{true value} - \text{approximate value}|$

$$|E_D(f)| \leq \max_{\theta \in [a,b]} \frac{h}{2} |f^{"}(\theta)|$$

Example

Example1. Using Taylor series find the derivative of $f(x) = x^2$ at x=1, with $h = .1$. Also compute the error.

Other formulae

Backward Formula

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}$$

Central Formula

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0 - h)}{2h}$$

Similarly, we can drive (Second Derivative)

$$f''(x_0) \approx \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2}$$

Derivative for discrete data using interpolating polynomial

x	x_0	x_1	x_2	...	x_n
$f(x)$	$f(x_0)$	$f(x_1)$	$f(x_3)$	...	$f(x_n)$

Assumption: $x_0, x_1 \cdots x_n$ are equispaced i.e., $x_i - x_{i-1} = h$. Where the explicit nature of the function f is not known.

Remark 1: We can used Newton's Forward or Backward formula depends the location of the point

Remark 2: If data is not equispaced then Lagrange interpolating polynomial can be used.

Using Newton's forward difference formula

$$f(x) \approx P_n(x) = f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \frac{s(s-1)(s-2)}{3!}\Delta^3 f(x_0)$$
$$\cdots \frac{s(s-1)(s-2)\cdots(s-n+1)}{n!}\Delta^n f(x_0)$$

where

$$x = x_0 + sh$$

We use $p_n(x)$ to calculate the derivatives of f.

That is $f'(x) \simeq p_n'(x)$ for all $x \in [x_0, x_n]$.

For a given x,

$$f'(x) \simeq p_n'(x)$$

$$= \frac{dp_n}{ds}\frac{ds}{dx}$$

$$= \frac{1}{h}\frac{dp_n}{ds}$$

Similarly,

$$f''(x) \simeq \frac{d^2p_n}{dx^2}$$

$$\frac{d}{dx}(\frac{dp_n}{dx})$$

$$= \frac{d}{dx}(\frac{dp_n}{ds}\frac{ds}{dx})$$

$$= \frac{1}{h}\frac{d}{dx}(\frac{dp_n}{ds})$$

$$= \frac{1}{h}\left(\frac{d^2 p_n}{ds^2}\frac{1}{h}\right)$$
$$= \frac{1}{h^2}\frac{d^2 p_n}{ds^2}$$

Thus in general,

$$f^{(k)}(x) = \frac{1}{h^k}\frac{d^k p_n}{ds^k}$$

Example 1

Using Taylor series expansion (forward formula) and Newton forward divided difference, compute first and second derivative at $x = 2$ for the following tabulated function

x	1	2	3	4
$f(x)$	2	5	7	10

Solution

x	$f(x)$	Δ	Δ^2	Δ^3
1	2			
		3		
2	5		-1	
		2		2
3	7		1	
		3		
4	10			

Here $h = 1$ Using Taylor series

$$f'(2) = \frac{f(2+h) - f(2)}{h} = \frac{f(3) - f(2)}{1} = 2$$

$$f''(2) = \frac{f(2+h) - 2f(2) + f(2-h)}{h^2} = \frac{f(3) - 2f(2) + f(1)}{1} = -1$$

Using Newton forward divided difference formula

$$f(x) \approx P_n(x) = f(x_0)+s\Delta f(x_0)+\frac{s(s-1)}{2!}\Delta^2 f(x_0)+\frac{s(s-1)(s-2)}{3!}\Delta^3 f(x_0)$$

$$f'(x) \approx \frac{1}{h}\frac{dp_n}{ds} = \frac{1}{h}\left[\Delta f(x_0) + \frac{2s-1}{2!}\Delta^2 f(x_0) + \frac{3s^2-6s+2}{3!}\Delta^3 f(x_0)\right]$$

Here $x = 2$, $x_0 = 1$, $s = 1$ and $h = 1$

$$f'(2) = 3 - \frac{1}{2} - \frac{1}{3} = 13/6$$

$$f''(x) \approx \frac{1}{h^2}\frac{d^2p_n}{ds^2} = \frac{1}{h^2}\left[\Delta^2 f(x_0) + (s-1)\Delta^3 f(x_0)\right]$$

$$f''(2) = -1$$

Example 2

Calculate $f^{(4)}(0.15)$

x	0.1	0.2	0.3	0.4	0.5	0.6
$f(X)$	0.425	0.475	0.400	0.450	0.525	0.575

Solution:

Newton's forward difference formula:

$$p_5(x) = f(x_0) + s\triangle^1 f(x_0) + \frac{s^2 - s}{2}\triangle^2 f(x_0) + \frac{s^3 - 3s^2 + 2s}{6}\triangle^3 f(x_0) +$$

$$+\frac{s^4 - 6s^3 + 11s^2 - 6s}{24}\triangle^4 f(x_0) + \frac{s^5 - 10s^4 + 35s^3 - 50s^2 + 24s}{120}\triangle^5 f(x_0)$$

Differentiating this 4-times we get,

$$\frac{d^4 f}{dx^4} \simeq \frac{dp_5^4}{dx^4} = \frac{1}{h^4}[\triangle^4 f(x_0) + \frac{1}{5}(5s - 10)\triangle^5 f(x_0)$$

$$= \frac{1}{h^4}[\triangle^4 f(x_0) + (s - 2)\triangle^5 f(x_0)]$$

$$= \frac{1}{(0.1)^4}[-035 + (0.5 - 2)(0.4)] = -95.00 \times 10^2$$

x	$f(x)$	$\triangle^1 f$	$\triangle^2 f$	$\triangle^3 f$	$\triangle^4 f$	$\triangle^5 f$
0.1	0.425					
		0.050				
0.2	0.475		-0.125			
		-0.075		0.25		
0.3	0.400		0.125		-0.35	
	‘	0.050		-0.100		0.4
0.4	0.450		0.025		0.05	
		0.075		-0.05		
0.5	0.525		-0.025			
		0.050				
0.6	0.575					

Numerical Integration

If $f : [a,b] \longrightarrow R$ is differentiable then, we obtain a new function $f' : [a,b] \longrightarrow R$, called the derivative of f. Likewise, if $f : [a,b] \longrightarrow R$ is integrable, then we obtain a new function $F : [a,b] \longrightarrow R$ defined by

$$F(x) = \int_a^x f(t)dt \qquad \forall x \in [a,b].$$

Observation: If f is nonnegative function, then $\int_a^b f(x)dx$ is represent the area under the curve $f(x)$.

Antiderivative

Antiderivative: Let $F : [a, b] \longrightarrow R$ be such that $f = F'$, then F is called an antiderivative of f.

Recall

Fundamental Theorem of Calculus: Let $f : [a, b] \longrightarrow R$ is integrable and has an antiderivative F, then

$$\int_a^b f(x)dx = F(b) - F(a).$$

Basic Problems

- Difficult to find an antiderivative of the function (for example $f(x) = e^{-x^2}$)

- Function is given in the tabular form.

Newton-Cotes Methods/Formulae

The derivation of Newton-Cotes formula is based on Polynomial Interpolation.

x	x_0	x_1	x_2	...	x_n
$f(x)$	$f(x_0)$	$f(x_1)$	$f(x_3)$	...	$f(x_n)$

The idea is:

Replace f by $p_n(x)$ and evaluate $\int_a^b p_n(x)dx$

That is,

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

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

$$= \sum_{i=0}^{n} A_i f(x_i)$$

Where $A_i = \int_a^b l_i(x)dx$ called weights.

Types of Newton-Cotes Formulae

- Trapezoidal Rule (Two pint formula)
- Simpson's $1/3$ Rule (Three Point formula)
- Simpson's $3/8$ Rule (Four point formula)

Trapezoidal Rule

Since it is two point formula, it uses the first order interpolation polynomial $P_1(x)$.

$$\int_a^b f(x) \approx \int_{x_0}^{x_1} P_1(x)dx$$

$$P_1(x) = f(x_0) + s\Delta f(x_0)$$

$$s = \frac{x - x_0}{h}$$

Now, $dx = h\ ds$ at $x = x_0, s = 0$ and at $x = x_1, s = 1$.

Hence,

$$\int_a^b f(x)dx \approx \int_0^1 (f(x_0) + s\Delta f(x_0))h ds = \frac{h}{2}[f(x_0) + f(x_1)]$$

OR

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

Error

$$E^T = -\frac{(b-a)^3}{12} f''(\xi),$$

where $a < \xi < b$

Remark: $x_0 = a$ and $x_1 = b$.

Basic Simpson's $\frac{1}{3}$ Rule

To evaluate $\int_a^b f(x)dx$.

- f will be replaced by a polynomial of degree 2 which interpolates f at a, $\frac{a+b}{2}$ and b. . Here, $x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b$

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

Error

$$E^s = \frac{-h^5 f^{(4)}(\xi)}{90}$$

for some $\xi \in (a, b)$.

Basic Simpson's $\frac{3}{8}$ Rule

- f is replaced by $p_3(x)$ which interpolates f at $x_0 = a, \quad x_1 = a + h, \quad x_2 = a + 2h, \quad x_3 = a + 3h = b$. where $h = \frac{b-a}{3}$. Thus we get:

$$\int_a^b f(x)dx \simeq \frac{3h}{8}[f_0 + 3f_1 + 3f_2 + f_3]$$

Error: $E^s = \dfrac{-3h^5}{80} f^{(4)}(\xi)$, where $a < \xi < b$.

Example

Using Trapezoidal and Simpson $\frac{1}{3}$ rules find $\int_0^2 x^4 dx$ and $\int_0^2 sinx dx$ and find the upper bound for the error.

Composite Rules

Note that if the integral $[a, b]$ is large, then the error in the Trapezoidal rule will be large.

Idea

Error can be reduced by dividing the interval $[a, b]$ into equal subinterval and apply quadrature rules in each subinterval.

Composite Trapezoidal Rule

$$h = \frac{b-a}{n}, \quad x_i = x_0 + ih$$

Composite Rule

$$\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)dx$$

Now apply Trapezoidal rule on each $[x_{i-1}, x_i]$, we have

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(x_0) + 2 * (f(x_1) + f(x_2) \cdots f(x_{n-1})) + f(x_n)\right]$$

Error in composite Trapezoidal rule

$$E^{CT} = -(b-a)\frac{h^2}{12}f^{''}(\xi), \;\; \xi \in [a,b]$$

The Composite Simpson's $\frac{1}{3}$ Rule

- $[a, b]$ will be will be divided into $2n$ equal subintervals and we apply basic Simpson's $\frac{1}{3}$ rule on each of the n intervals $[x_{2i-2}, x_{2i}]$ for $i = 1, 2, 3, \cdots, n$.

Thus here $h = \frac{b-a}{2n}$.

Then

$$\int_a^b f(x)dx = \int_{a=x_0}^{b=x_{2n}} f(x)dx$$

$$= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{2i-2}}^{x_{2i}} f(x)dx + \cdots + \int_{x_{2n-2}}^{x_{2n}} f(x)dx$$

$$= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] + \frac{h}{3}[f(x_2) + 4f(x_3) + f(x_4)] +$$

$$+ \cdots + \frac{h}{3}[f(x_{2n-2}) + 4f(x_{2n-1}) + f(x_{2n})]$$

$$= \frac{h}{3}\{f(x_0) + 4 \times [f(x_1) + f(x_3) + f(x_5) + \cdots + f(x_{2n-1})] +$$

$$+2 \times [f(x_2) + f(x_4) + f(x_6) + \cdots + f(x_{2n-2})] + f(x_{2n})\}$$

$$E^{CS} = -(b-a)\frac{h^4}{180}f^{(4)}(\xi),$$

where $\xi \in [a, b]$

Example

Evaluate the integral $\int_{-1}^{1} x^2 \exp(-x)dx$ by composite Simpson's $\frac{1}{3}$ rule with spacing $h = 0.25$

Solution: According to composite Simpson's $\frac{1}{3}$ rule:

$$\int_{-1}^{1} x^2 \exp(-x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) +$$

$$+4f(x_5) + 2f(x_6) + 4f(x_7) + f(x_8)]$$

Here $f(x_0) = f(-1) = 2.7183$

$f(x_1) = f(-0.75) = 1.1908$

$$f(x_2) = f(-0.5) = 0.4122$$

$$f(x_3) = f(-0.25) = 0.0803$$

$$f(x_4) = f(0) = 0$$

$$f(x_5) = f(0.25) = 0.0487$$

$$f(x_6) = f(0.50) = 0.1516$$

$$f(x_7) = f(0.75) = 0.2657$$

$$f(x_8) = f(1) = 0.3679$$

Substituting these values in the above formula we get:

$$\int_{-1}^{1} x^2 \exp(-x)dx \simeq 0.87965$$

Example

Find the minimum no. of subintervals, used in composite Trapezoidal and Simpson's $1/3$ rule in order to find the integral $\int_0^1 e^{-x^4} dx$ such that the error can not exceed by $.00001$.

Sol. For the composite Trapezoidal rule, we have

$$\frac{1^3 \max_{0<\xi<1} |f^{''}(\xi)|}{12 n_{trap}^2} \leq .00001$$

For the composite Simpson $1/3$ rule, we have

$$\frac{1^4 \max_{0<\xi<1} |f^{(4)}(\xi)|}{180 n_{simp}^4} \leq .00001$$

Now,

$$\max_{0<\xi<1} |f^{''}(\xi)| \leq 3.5, \qquad \max_{0<\xi<1} |f^{(4)}(\xi)| \leq 95$$

(Please verify)

Hence

$$n_{trap} = 171, n_{simp} = 16$$

Composite Simpson's $\frac{3}{8}$ rule

- $[a, b]$ is divided into $3n$ equal subintervals. ($h = \frac{b-a}{3n}$. and we apply $\frac{3}{8}$ rule on each of the n **intervals** $[x_{3i-3}, x_{3i}]$ for $i = 1, 2, 3, \cdots, n$.)

Hence,

$$\int_a^b f(x)dx \simeq \int_{x_0=a}^{x_3} f(x)dx + \int_{x_3}^{x_6} f(x)dx + \cdots + \int_{x3n_3}^{x_{3n}=b} f(x)dx$$

$$= \frac{3h}{8}[f_0 + 3f_1 + 3f_2 + f_3] + \frac{3h}{8}[f_3 + 3f_4 + 3f_5 + f_6] +$$

$$+ \cdots + \frac{3h}{8}[f_{3n-3} + 3f_{3n-2} + 3f_{3n-1} + f_{3n}]$$

$$= \frac{3h}{8}[f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + 3f_7 + \cdots + 3f_{3n-1} + f_{3n}]$$

Remember:

- f with suffices of multiple 3 are multiplied by 2.
- Others by 3, *except the end points*.

Example

Use composite simpson's $\frac{3}{8}$ rule, find the velocity after 18 seconds, if a rocket has acceleration as given in the table:

$t =$	0	2	4	6	8	10	12	14	16	18
$a =$	40	60	70	75	80	83	85	87	88	88
	f_0	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9

Sol: Velocity $v = \frac{3h}{8}[f_0+3f_1+3f_2+2f_3+3f_4+3f_5+2f_6+3f_7+3f_8+f_9]=$ $\frac{3}{4}[40+3\times60+3\times70+2\times75+3\times80+383+2\times83+2\times85+3\times87+3\times88+88]$

$$= 1389 \quad units.$$

Method of Undetermined Parameters

The Newton - Cotes integration rules are all of the form

$$I(f) \simeq A_0 f(x_0) + A_1 f(x_1) + A_2 f(x_2) + \cdots + A_n f(x_n)$$

Also, note that the weights A_i's do not depend on the given function.

Hence, if the error is of the form

$$E(I) = Const \times f^{(r+1)}(\eta).$$

Then the rule must be exact for all polynomials of degree $\leq r$

Therefore

If we wish to construct a rule of the form

$$I(f) \simeq A_0 f(x_0) + A_1 f(x_1) + a_2 f(x_2) + \cdots + A_n f(x_n)$$

(n-fixed) which is exact for polynomials of degree as high as possible, i.e., we want

$$E(I) = Const \times f^{(r+1)}(\eta),$$

with r as large as possible.

This way of constructing integration rules is called the " Method of Undetermined Parameters".

Example

Suppose we want to derive an integration formula of the form:

$\int_a^b f(x)dx = A_0\ f(a) + A_1\ f(b) + \alpha\ f''(\xi).$

We assume that: The rule is exact for the polynomials $1,\ x, x^2$.

Now, taking $f(x) = 1$, we get $b - a = A_0 + A_1$

Taking $f(x) = x$ we get $\frac{b^2 - a^2}{2} = A_0 a + A_1 b$

Solving the above two equations we get, $A_0 = A_1 = \frac{b-a}{2}$.

Thus, $\displaystyle\int_a^b f(x)dx = \frac{b-a}{2}[f(a) + f(b)] + \alpha\ f''(\xi)$

Now if we take $f(x) = x^2$, we get:

$$\frac{b^3 - a^3}{3} = (\frac{b-a}{2})(a^2 + b^2) + 2!\ \alpha$$

$$\implies \alpha = -\tfrac{(b-a)^3}{12}$$

Thus

$$\int_a^b f(x)dx = \frac{b-a}{2}[f(a) + f(b)] - \frac{(b-a)^3}{12}\ f''(\xi)$$

We see that: This is exactly the trapezoidal rule. **Similarly**, Simpson's $\frac{1}{3}$ and $\frac{3}{8}$ rules can be derived.

Thus in the Method of Undetermined Parameters

• We aim directly for a formula of a preselected type.

Working Method:

• We impose certain conditions on a formula of desired form and use these conditions to determine the values of the unknown coefficients in the formula.

The Error term in the Simpson's $\frac{3}{8}$-rule, using Method of Undetermined Parameters

Start with:

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}[f_0 + 3f_1 + 3f_2 + f_3] + \alpha\ f^{(4)}(\xi)$$

for some suitable $\xi \in (x_0, x_3)$.

Takeing $f(x) = x^4$ in the above integration rule we get:

$$\frac{x_3^5 - x_0^5}{5} = \frac{3h}{8}[x_0^4 + 3x_1^4 + 3x_2^4 + x_3^4] + \alpha\ 4!$$

$$4!\alpha = \frac{x_3^5 - x_0^5}{5} - \frac{3h}{8}[x_0^4] + 3(x_0+h)^4 + 3(x_0+2h)^4 + (x_0+3h)^4$$

$$= \frac{(x_0+3h)^5 - x_0^5}{5} - \frac{3h}{8}[x_0^4] + 3(x_0+h)^4 + 3(x_0+2h)^4 + (x_0+3h)^4$$

Without loss of generality, we can take: $x_0 = 0.$

We have: $4!\alpha = \frac{243}{5}h^5 - \frac{3h^5}{8}[0 + 3 + 3 \times 16 + 81]$ Thus

$$4!\alpha = -\frac{9}{10}h^5$$

That is,

$$\alpha = -\frac{3}{80}h^5$$

Therefore the error in the Simpson's rule is =

$$-\frac{3}{80}h^5\, f^{(4)}(\xi)$$

for some suitable $\xi \in (a, b)$.

Recall

The Newton - Cotes integration rules are all of the form

$$I(f) \simeq A_0 f(x_0) + A_1 f(x_1) + A_2 f(x_2) + \cdots + A_n f(x_n)$$

Also, note that the weights A_i's do not depend on the given function.

Hence, if the error is of the form $E(I) = Const \times f^{(r+1)}(\eta)$. Then the rule must be exact for all polynomials of degree $\leq r$.

Remark: In these quadrature the points x_i are fixed.

Ques: Can we improve the accuracy by choosing some suitable x_i

Ans: Using Gaussian Quadrature rule one can improve the accuracy.

Example

Find x_0, x_1, A_0, A_1 and α so that the following rule is exact for all polynomials of degree≤ 3.

$$\int_{-1}^{1} f(x)dx = A_0 f(x_0) + A_1 f(x_1) + \alpha f^{(4)}(\xi)$$

(There are 4 unknowns and hence we have chosen the 4-th derivative in the error term.)

Taking $f(x) = 1, x, x^2, x^3$ we get:

$A_0 + A_1 = 2$

$A_0x_0 + A_1x_1 = 0$

$A_0x_0^2 + A_1x_1^2 = \frac{2}{3}$

$A_0x_0^3 + A_1x_1^3 = 0$

On solving these equations we get:

$A_0 = A_1 = 1$ $x_0 = -\frac{1}{\sqrt{3}}$ and $x_1 = \frac{1}{\sqrt{3}}$.

Thus the integration rule is: $\int_{-1}^{1} f(x)dx = f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) + \alpha f^{(4)}(\xi)$.

Now if we take $f(x) = x^4$ we get

$$\frac{2}{5} = \frac{2}{9} + \alpha 4!$$

$$\implies \alpha = \frac{1}{4!}(\frac{8}{45}) = \frac{1}{135}$$

Thus the expected integration rule is:

$$\int_{-1}^{1} f(x)dx = f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) + \frac{1}{135} f^{(4)}(\xi).$$

In general

Giving a positive integer n, we wish to determine $2n+2$ numbers $x_0, x_1, \cdots x_n$ and $A_0, A_1, \cdots, A_n$ so that the sum

$$I(f) \simeq A_0 f(x_0) + A_1 f(x_1) + A_2 f(x_2) + \cdots + A_n f(x_n),$$

provides the exact value of $\int_a^b f(x)dx$ for $f(x) = 1, x, x^2, \cdots x^{2n+1}$.

Or What we want is that the quadrature rule is exact for all polynomials of degree $\leq 2n+1$.

Remark: Here we have to solve system of nonlinear equations, which is some time is not an easy job.