PROGRAM ROZWOJOWY
POLITECHNIKI WARSZAWSKIEJ

LECTURE 3

NUMERICAL INTEGRATION

KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

UNIA EUROPEJSKA
EUROPEJSKI
FUNDUSZ SPOŁECZNY

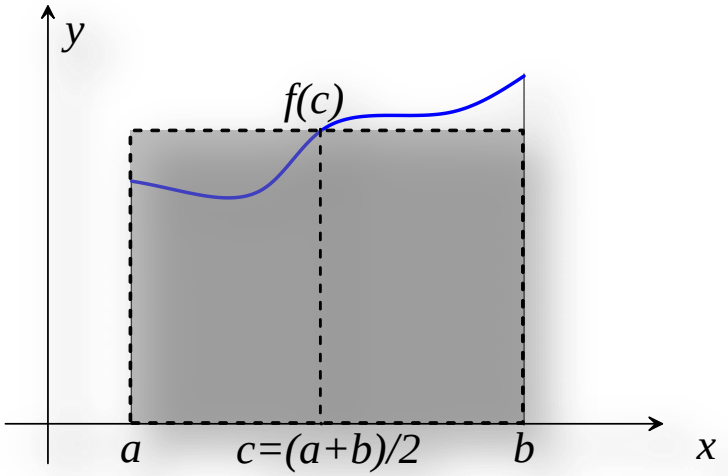
Numerous definite integrals an engineer may encounter in practice cannot be calculated by hand. Some others can, but the calculations are extremely tedious. In both cases, it seems reasonable to use some numerical technique instead, which delivers an approximate value of the integral. In other words – let the computer does the job!

In this lecture, we will explore some of the most basic numerical integration algorithms. Here, the discussion will be limited to regular definite integral of the functions of a single variable. Hence, we will be interested in the algorithms of approximate evaluation of the integral

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

where the function f is continuous in the closed interval $[a,b]$ (note that f is automatically bounded in this interval). The method of numerical integration will be referred to as **integrations rules** or **quadratures**.

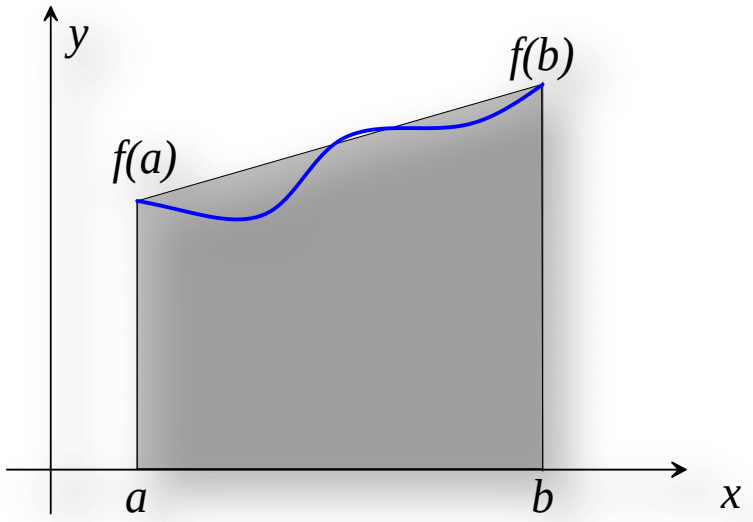
MID-POINT (M) INTEGRATION RULE



The first integration method to discuss is the mid-point rule. Its idea is very simple – see the figure. Thus, the formula can be written as

$$I \approx I_M = (b-a)\, f(c) \quad , \quad c = (a+b)/2$$

TRAPEZOIDAL (T) INTEGRATION RULE

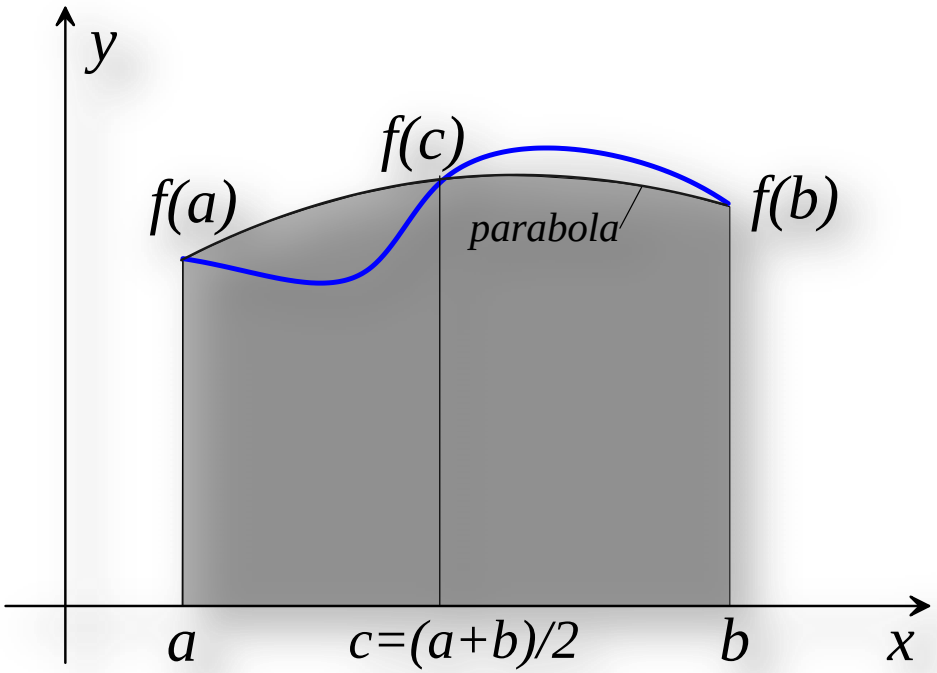


Another possibility is to approximate the integral I by the trapezoidal formula (the name is obvious – see figure on the left). The corresponding formula reads

$$I_T = \tfrac{1}{2}(b-a)[\, f(a) + f(b)]$$

Thus, we approximate f by the **linear function** and integrate analytically.

SIMPSON (S) INTEGRATION RULE



Yet another simple method consists in approximating the function f by the second-order interpolating polynomial. The nodes are the midpoint and both ends of the integration interval. Then, the polynomial is integrated analytically. One obtains the formula

$$I_S = \frac{1}{6}(b-a)[f(a)+4f(c)+f(b)]$$

where $c = (a + b)/2$.

THE NEWTON-COTES RULES

The idea behind the trapezoidal and Simpson rules is to approximate the integrated function by the interpolating polynomial. This idea can be generalized to higher orders by introducing larger number of the nodal points inside the integration interval. Then the value of the integral is evaluated from the formula

$$I(f) \equiv \int_a^b f(x)dx \approx \int_a^b P_n(x)dx \equiv I_n(f)$$

In the above, the symbol P_n denotes the nth-order interpolating polynomial. We know that such polynomial can be expressed as the linear combination of special Lagrange polynomials (see Lecture 1)

$$P_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x)$$

Thus, the general Newton-Cotes rule has the form

$$I_n(f) = \sum_{k=0}^{n} \underbrace{\left(\int_a^b l_k(x)dx \right)}_{\alpha_k} f(x_k) = \sum_{k=0}^{n} \alpha_k \; f(x_k)$$

ACCURACY OF THE INTEGRATION RULES

Let us discuss shortly the issue of accuracy of the numerical integration. Consider first the **midpoint rule**. Using the Taylor theorem we can write

$$f(x) = f(c) + f'(c)(x-c) + \tfrac{1}{2} f''(\hat{x})(x-c)^2 \quad , \quad \hat{x} \in [a,b]$$

Integrating both sides of the above equality we get

$$\int_a^b f(x)dx = \underbrace{(b-a) f(c)}_{I_M} + f'(c) \underbrace{\int_a^b (x - \tfrac{a+b}{2})dx}_{0} + \tfrac{1}{2}\int_a^b f''[\hat{x}(x)](x-c)^2 dx =$$

$$= I_M + \tfrac{1}{24} f''(\xi)(b-a)^3$$

For the last term we have used the mean-value theorem, namely

$$\int_a^b f''[\hat{x}(x)] \underbrace{(x-c)^2}_{\text{nonnegative in } [a,b]} dx \underset{\substack{\Uparrow \\ \text{mean-value} \\ \text{theorem}}}{=} f''[\underset{\substack{\Uparrow \\ \text{some point} \\ \text{in } [a,b]}}{\xi}] \int_a^b (x-c)^2 dx =$$

$$= \tfrac{1}{12} f''(\xi)(b-a)^3$$

Analogous analysis for the trapezoidal rule is carried out as follows. First, using the result proven in the **Lecture 1** we can write

$$f(x) = P_1(x) + \tfrac{1}{2} f''[\hat{x}(x)](x-a)(x-b)$$

Here, P_1 is the linear function which interpolates the endpoint values of the function *f*. The integration of the above equality yields

$$\int_a^b f(x)dx = I_T(f) + \tfrac{1}{2}\int_a^b f''[\hat{x}(x)]\underbrace{(x-a)(x-b)}_{\text{nonpositive in } [a,b]}dx =$$

$$= I_T(f) + \tfrac{1}{2} f''(\xi)\int_a^b (x-a)(x-b)dx = I_T(f) - \tfrac{1}{12} f''(\xi)(b-a)^3$$

Note that we have obtained consistent result: the trapezoidal rule overestimates the value of the integral of a convex functions ($f'' > 0$) and underestimates the value of the integral of a concave function ($f'' < 0$).

The accuracy analysis of the Simpson method can be performed in the similar way (however, it is more laborious). The following estimate can be obtained

$$\int_a^b f(x)dx = I_S(f) - \frac{1}{2880} f^{IV}(\xi)(b-a)^5$$

Note that the error expression for the midpoint and trapezoidal rules contains the value of the second derivative of the integrated function in some intermediate point. It is consistent with the obvious observation that both methods are exact for any linear function. On the other hand, they are not exact for the second-order polynomials. We say that midpoint and trapezoidal rules are the **first-order** methods. The error estimation of the Simpson rule contains the 4^{th}-order derivative of the function f. This means that this method is exact for all polynomials of the order not larger than 3. Hence, **the Simpson rule is of the third order**.

In general, the order of the Newton-Cotes rules (closed, i.e. using both endpoints as the interpolation nodes) based on the n^{th}-order interpolation (n + 1 points are used) is equal n if n is odd (1,3,..) or n + 1 if n is even (2,4,..).

COMPOSITE INTEGRATION RULES

Significant improvement of accuracy of the numerical integration can be obtained by using the composite rules. The idea is simple: instead of using any of the above mentioned rules for the whole interval [*a*,*b*] we use it for a number of smaller subintervals and in the end we summate the contributions. In other words, if we have the subdivision of the interval described as

$$a = x_0 < x_1 < x_2 < \ldots < x_{n-1} < x_n = b$$

then

$$I = \int_a^b f(x)dx = \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} f(x)dx$$

The **composite midpoint rule** (**CMR**) consists in evaluation of each integral in the above sum by means of the (simple) midpoint formula. Thus

$$I \approx I_M^n(f) = \sum_{k=0}^{n-1} f(c_k)(x_{k+1} - x_k) \quad , \quad c_k = (x_k + x_{k+1})/2 \ , \ k = 0,1,..,n-1$$

If the interval $[a,b]$ is divided into n **equal subintervals** then the composite midpoint rule can be written as

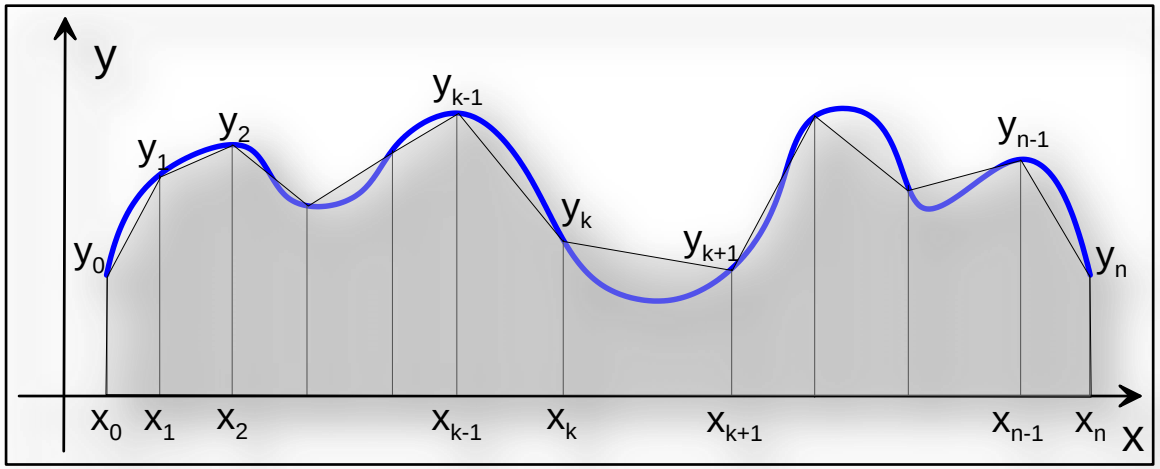
$$I_M^n(f) = h\sum_{k=0}^{n-1} f(c_k) \quad , \quad h=(b-a)/n \ , \ c_k = x_k + h/2 = a + (k+\tfrac{1}{2})h \ , \ k=0,1,..,n-1$$

It can be shown that the error of the CMR can be expressed by the formula

$$E_M^n = \int_a^b f(x)dx - I_M^n = \tfrac{1}{24} f''(\xi)(b-a)h^2 \quad , \quad \xi \in [a,b]$$

Again, we conclude that CMR is exact for any linear function. Obviously, it is also exact for any piecewise-linear function providing that the division to subintervals matches the “pieces”. But what is even more important, the integration error shrinks with increasing number of subintervals. In particular, for the uniform division the error diminishes as quick as h^2.

In the similar manner (see figure), one can define the **composite trapezoidal rule (CTR)**.



Its general formula is

$$I \approx I_T^n(f) = \sum_{k=0}^{n-1} \tfrac{1}{2}[f(x_k) + f(x_{k+1})](x_{k+1} - x_k)$$

For the uniformly distributed nodes one gets

$$I_T^n(f) = \left[\tfrac{1}{2} f(x_0) + \sum_{k=1}^{n-1} f(x_k) + \tfrac{1}{2} f(x_0) \right] h$$

and the error formula is

$$E_T^n = \int_a^b f(x)dx - I_T^n = -\tfrac{1}{12} f''(\xi)(b-a)h^2 \quad , \quad \xi \in [a,b]$$

Thus, the CTR is basically as good as the CMR. However, the CTR is particularly useful for smooth periodic functions when the length of the integration interval is equal to the period. It can be shown (using the Euler-McLaurin formula) that in such case the error of the CTR shrinks to zero faster than any power of the distance *h*! We say that in such circumstances the CTR method attains **spectral convergence rate**.

Finally, the **composite Simpson rule (CSR)** reads

$$I_S^n(f) = \sum_{k=0}^{n-1} \tfrac{1}{6}[f(x_k) + 4f(c_k) + f(x_{k+1})](x_{k+1} - x_k) \quad , \; c_k = \tfrac{1}{2}(x_k + x_{k+1}) \; , \; k = 0,1,..,n-1$$

Again, for the equidistant nodes, the above formula can be re-written as

$$I_S^n(f) = \tfrac{1}{3}h\left[f(x_0) + 2\sum_{k=1}^{n-1} f(x_{2k}) + 4\sum_{k=0}^{n-1} f(x_{2k+1}) + f(x_{2n}) \right],$$

$$x_j = a + jh \; , \; j = 0,1,..,2n \; , \; h = \frac{b-a}{2n}$$

The corresponding error estimate has the following form

$$E_S^n = \int_a^b f(x)dx - I_S^n = -\frac{1}{180} f^{IV}(\xi)(b-a)h^4 \quad , \quad \xi \in [a,b]$$

We see that this time the error reduces proportionally to the 4^{th} power of the distance *h*. For majority of the practical application the CSR provides satisfactory level of accuracy with a reasonable number of nodes. However, further improvement of accuracy may be achieved by using the **recursive Romberg integration**.

GAUSS-LEGENDRE INTEGRATION

We will discussed an alternative and very popular method of approximate evaluation of the integrals – the Gauss-Legendre Method (GLM). The following calculation shows that it is sufficient to formulate this method (actually – any method) for the integral in the standard interval [-1,1]:

$$\int_a^b f(x)dx = \left| \begin{array}{c} x = \frac{1}{2}a(1-t) + \frac{1}{2}b(1+t) \;\; , \;\; dx = \frac{1}{2}(b-a)dt \\ x = a \Rightarrow t = -1 \quad , \quad x = b \Rightarrow t = 1 \end{array} \right| = \frac{1}{2}(b-a)\int_{-1}^{1} F(t)dt$$

In the above $$F(t) = f[\frac{1}{2}a(1-t) + \frac{1}{2}b(1+t)]$$

In order to derive an example of the GLM consider the following formula

$$\int_{-1}^{1} F(x)dx \approx w_1 F(x_1) + w_2 F(x_2) \;\; , \;\; x_1, x_2 \in [-1,1]$$

We need to find x_1, x_2, w_1 and w_2 such that the above **formula is exact for the polynomials of the highest possible order**.

We test this formula against monomials of increasing order in order to obtain the system of equations for the unknown parameters of the GLM:

$$F(t) = 1 \;\Rightarrow\; \int_{-1}^{1} 1\,dx = 2 = w_1 + w_2$$

$$F(t) = x \;\Rightarrow\; \int_{-1}^{1} x\,dx = 0 = w_1 x_1 + w_2 x_2$$

$$F(t) = x^2 \;\Rightarrow\; \int_{-1}^{1} x^2\,dx = \tfrac{2}{3} = w_1 x_1^2 + w_2 x_2^2$$

$$F(t) = x^3 \;\Rightarrow\; \int_{-1}^{1} x^3\,dx = 0 = w_1 x_1^3 + w_2 x_2^3$$

The equations for x_1, x_2, w_1 and w_2 are:

$$(a)\; w_1 + w_2 = 2$$

$$(b)\; w_1 x_1 = -w_2 x_2$$

$$(c)\; w_1 x_1^2 + w_2 x_2^2 = \tfrac{2}{3}$$

$$(d)\; w_1 x_1^3 = -w_2 x_2^3$$

The solution of the obtained equations is obtained as follows

$$x_1^2 = x_2^2 \quad and \quad x_1 \neq x_2 \quad \Rightarrow \quad x_1 = -x_2$$

$$w_1 = w_2 \quad \Rightarrow \quad w_1 = w_2 = 1$$

$$w_1 x_1^2 + w_2 x_2^2 = 2x_1^2 = \tfrac{2}{3} \quad \Rightarrow \; x_1^2 = \tfrac{1}{3} \; \Rightarrow \; x_1 = -x_2 = \tfrac{\sqrt{3}}{3} \approx 0.5773502692$$

Thus, the final Gauss-Legendre formula reads

$$\int_{-1}^{1} F(x)dx = F(-\tfrac{\sqrt{3}}{3}) + F(\tfrac{\sqrt{3}}{3}) + E_2(F)$$

Note that this formula is exact for any polynomial of the order not larger than 3. In fact, the following error estimate can be derive

$$E_2(F) = \tfrac{1}{135} F^{IV}(\xi)$$

GENERAL APPROACH TO GAUSS QUADRATURES

Similarly to the Newton-Cotes rules, the Gauss integration methods use the interpolation polynomials to approximate the integrated function. However, the interpolation nodes are chosen in a special way which guarantees the highest possible order of accuracy. The way these nodes are selected is strictly related to the **concept of orthogonal polynomials**.

Consider the standard interval [-1,1]. Let the function **Ω**, positive and integrable in [-1,1], is given. We say that the given set of the polynomials

$$\{p_k(x) = a_{k,k}x^k + a_{k,k-1}x^k + \ldots + a_{k,0},\ k = 0,1,2,\ldots\}$$

is **Ω-orthogonal** in the interval [-1,1] if

$$\int_{-1}^{1} p_i(x)\,p_j(x)\Omega(x)dx = 0 \quad , \quad i \neq j$$

Two important examples are:

1. **Chebyshev polynomials**

We already (see Lecture 2) know that these polynomials are defined by the recurrence formula

$$T_0(x) = 1 \ , \ T_1(x) = x \ , \ T_{j+1}(x) = 2xT_j(x) - T_{j-1} \ , \ j = 1,2,..$$

The Chebyshev polynomials are Ω-orthogonal in the following sense

$$\int_{-1}^{1} T_i(x)T_j(x)\Omega(x)dx = \begin{cases} \pi \ , \ i = j = 0 \\ \frac{1}{2}\pi \ , \ i = j > 0 \\ 0 \ , \ i \neq j \end{cases}$$

where the weight function Ω is

$$\Omega(x) = \frac{1}{\sqrt{1-x^2}}$$

2. Legendre polynomials

The Legendre polynomials are defined by the following recurrent formula

$$L_0(x)=1\ ,\ L_1(x)=x\ ,\ L_{j+1}(x)=\frac{2j+1}{j+1}xL_j(x)-\frac{j}{j+1}L_{j-1}(x)\ ,\ \ j=1,2,..$$

or they can be expressed explicitly as

$$L_j(x)=\frac{1}{2^j}\sum_{k=0}^{[j/2]}(-1)^k\binom{j}{k}\binom{2j-2k}{j}x^{j-2k}\quad ,\quad j=0,1,2,...$$

They are also simply orthogonal in [-1,1], i.e., the weight function $\Omega \equiv 1$

$$\int_{-1}^{1}L_i(x)L_j(x)dx=\begin{cases}0 & ,\ \ i\neq j\\ \frac{2}{2i+1} & ,\ \ i=j\end{cases}$$

The general Gauss integration rule is design to evaluate the integral of the form

$$I_{\Omega}(f) = \int_{-1}^{1} f(x)\Omega(x)dx$$

Such rule can be written as

$$I_{n,\omega}(f) = \sum_{j=0}^{n} \alpha_j f(x_j) \quad , \quad x_j \in [-1,1] \ , \ j = 0,1,..,n$$

The coefficients are computed from the following integrals

$$\alpha_j = \int_{-1}^{1} l_j(x)\Omega(x)dx = \int_{-1}^{1} \frac{(x-x_0)\ldots(x-x_{j-1})(x-x_{j+1})\ldots(x-x_n)}{(x_j-x_0)\ldots(x_j-x_{j-1})(x_j-x_{j+1})\ldots(x_j-x_n)}\Omega(x)dx$$

where $l_j(x),\ j = 0,..,n$ are the Lagrange polynomials defined in the **Lecture 1**.

How should we choose the nodes of the Gauss quadrature? The key result (proven by **Carl Jacobi** in 1826) is:

The order of the interpolation quadrature based on *n* +1 nodes (thus, using interpolation by nth-order polynomial) is *n* + *m* if and only if the polynomial

$$\upsilon_{n+1}(x) = (x - x_0)\ldots(x - x_{j-1})(x - x_{j+1})\ldots(x - x_n)$$

satisfies the following conditions

$$\int_{-1}^{1} x^k \upsilon_{n+1}(x)\Omega(x)dx = 0 \quad , \quad k = 0,1,..,m-1$$

Remark: Clearly, the polynomial υ_{n+1} is automatically Ω-orthogonal to all polynomials with the order not exceeding *m*-1.

Proof:

Assume that f is the $(n+m)^{\text{th}}$-order polynomial. Then, it can be written in the form

$$f(x) = \upsilon_{n+1}(x) q_{m-1}(x) + r_n(x)$$

Since the order of the polynomial r_n is at most equal n, then the application of the integration rule brings an exact value of the integral. Thus, we have

$$\sum_{j=0}^{n} \alpha_j r_n(x_j) \equiv \int_{-1}^{1} r_n(x)\Omega(x)dx = \int_{-1}^{1} f(x)\Omega(x)dx - \int_{-1}^{1} \upsilon_{n+1}(x) q_{m-1}(x)\Omega(x)dx$$

Now, due to the postulated property of the polynomial υ_{n+1} the equality holds

$$\int_{-1}^{1} \upsilon_{n+1}(x) q_{m-1}(x)\omega(x)dx = 0$$

Using the fact that $f(x_j) = r_n(x_j), \;\; j = 0,..,n$ we finally get the conclusion

$$\int_{-1}^{1} f(x)\omega(x)dx = \sum_{j=0}^{n} \alpha_j r_n(x_j) = \sum_{j=0}^{n} \alpha_j f(x_j)$$

The further conclusion is:

The maximal order of the interpolation quadrature based on *n* +1 nodes is equal 2*n*+1 (twice the number of the nodes minus one).

Indeed, assume the opposite, i.e. let the postulated orthogonality condition hold for $m = n+2$. Then, it follows that the polynomial υ_{n+1} is Ω-orthogonal to all polynomials of the order equal n+1. It means that in particular

$$\int_{-1}^{1} \upsilon_{n+1}^2(x)\omega(x)dx = 0$$

But this would be possible only if $\upsilon_{n+1}(x) \equiv 0$, which is not the case.

So what is the choice of the nodes which corresponds to the **most accurate quadrature**?

The maximal order of the GL integration rule is achieved when the polynomial υ_{n+1} is Ω-orthogonal to all polynomials of the order equal n , i.e.,

$$\int_{-1}^{1} \upsilon_{n+1}(x)\, p(x)\omega(x)dx = 0 \quad , \quad p \in \mathcal{P}_n$$

In particular, if $\Omega(x) \equiv 1$ this polynomial in simply the Legendre polynomial L_{n+1}:

$$\upsilon_{n+1}(x) = L_{n+1}(x) \;\Rightarrow\; x_j = \xi_j \;,\; j = 0,1,..,n$$

The nodes of the Gauss-Legendre quadrature are simply the roots of the Legendre polynomial L_{n+1}!

Summarizing, we have the formula $$\int_{-1}^{1} f(x)dx \approx I_{GL}(f) = \sum_{j=0}^{n} \alpha_j f(\xi_j)$$

The coefficient can be expresses as $$a_j = \frac{2}{(1-\xi_j^2)[L'_{n+1}(\xi_j)]^2} \quad , \quad j = 0,1,..,n$$

The following error estimate can be derived

$$\int_{-1}^{1} f(x)dx - I_{GL}(f) = \frac{2^{2n+3}[(n+1)!]^4}{(2n+3)[(2n+2)!]^3} f^{(2n+2)}(\hat{x}) \;,\; \hat{x} \in (-1,1)$$

It is evident that the order of this quadrature is $2n+1$.

In general, the roots of Legendre polynomials and corresponding coefficients cannot be found analytically. However, they have been very accurately computed numerically for different values of *n*. Their values can be easily found in many handbooks or in the Internet.

Other kinds of the highly accurate Gauss integration methods can be design. In one wants to calculate the integral with the Chebyshev weight function, the appropriate method would be the Gauss-Chebyshev quadrature. There exist also other types of Gauss-like quadratures which are design to approximate integrals over different intervals and different weight functions **Ω**.

Note that if the actual interval of integration is different than the standard one, then one has to apply an appropriate (usually linear) **change of variable**. The details are left to the Reader.