Numerical analysis
Numerical integration

Kazuaki Tanaka

For $f \in C([a,b])$, calculating the integral

$F' = f$

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

is often important for many purposes. If we know the primitive function F of f, we can obtain the integral as

$$I = F(b) - F(a).$$

However, primitive functions are not always computable concretely. This is when the numerical integration method comes into play.

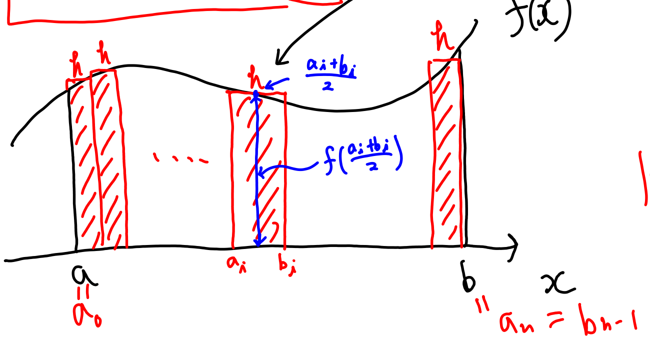
1 Rectangular rule

$$\boxed{I \sim \sum_{i=0}^{n-1} f\left(\frac{a_i+b_i}{2}\right) h}$$

$$\int_{a_i}^{b_i} f(x)\,dx \sim f\left(\frac{a_i+b_i}{2}\right)\cdot h$$

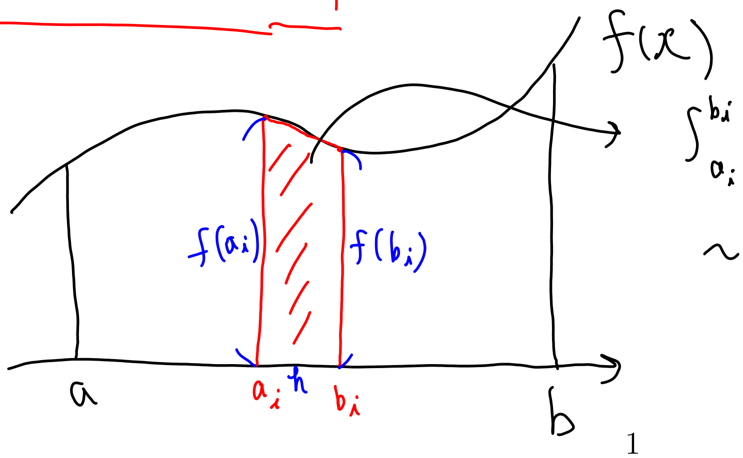
$$I \sim \sum_{i=0}^{n-1} f\left(\frac{a_i+b_i}{2}\right) h$$

$$\boxed{a_{i+1} = a_i + h}$$



2 Trapezoidal rule

$$\boxed{I \sim \sum_{i=0}^{n-1} \frac{h}{2} \left[f(a_i) + f(b_i)\right]}$$



$$\int_{a_i}^{b_i} f(x)\,dx \sim \frac{1}{2} h \left(f(a_i) + f(b_i)\right)$$

3 Error Analysis

$$I = \int_0^2 \sin x dx = 1 - \cos 2 = 1.416146 \cdots .$$

h	Rectangular error		Trapezoidal error
2^{-5}	5.7×10^{-5}	$<$	1.15×10^{-4}
2^{-6}	1.4×10^{-5}	$<$	2.88×10^{-5}
2^{-7}	3.6×10^{-6}	$<$	7.20×10^{-6}

$\div 2$ $\div 2$

$\div 4$ $\div 4$ $\div 4$ $\div 4$

$O(h^2)$?

For rectangular case

Let us define

$$E := \left| \overset{\text{exact}}{\int_a^b f(x)dx} - h \underbrace{\overset{\text{rectangular rule}}{\sum_{i=0}^{n-1} f(x_i)}}_{} \right|, \quad x_i = \frac{a_i + b_i}{2}$$

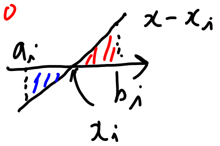
$$= \left| \sum_{i=0}^{n-1} \underbrace{\left(\int_{a_i}^{b_i} f(x)dx - hf(x_i) \right)}_{E_i} \right| = \left| \sum_{i=0}^{n-1} E_i \right| \overset{\text{triangle ineq.}}{\leq} \sum_{i=0}^{n-1} |E_i|$$

where $E_i = \int_{a_i}^{b_i} f(x)dx - hf(x_i)$. Using Taylor's theorem, we have

$$f(x) = f(x_i) + f'(x_i)(x - x_i) + \frac{1}{2} f''(t)(x - x_i)^2 \quad \text{for all } x \in [a_i, b_i],$$

where t lies between x and x_i. Integrating $f(x)$ from a_i to b_i, we have

$$\int_{a_i}^{b_i} f(x)dx = \underbrace{(b_i - a_i)}_{h} f(x_i) + f'(x_i) \underbrace{\cancel{\int_{a_i}^{b_i} (x - x_i)dx}}_{=0} + \frac{1}{2} \int_{a_i}^{b_i} f''(t)(x - x_i)^2 dx$$



$$= \underline{hf(x_i)} + \frac{1}{2} \int_{a_i}^{b_i} f''(t)(x - x_i)^2 dx.$$

$$E_i = \int_{a_i}^{b_i} f(x)\,dx - hf(x_i) = \frac{1}{2} \int_{a_i}^{b_i} f''(t)\,(x - x_i)^2 dx$$

Then, we get

$x \le t \le x_i$
or
$x_i \le t \le x$

$$\begin{aligned} |E_i| &= \left| \int_{a_i}^{b_i} f(x)dx - hf(x_i) \right| \\ &= \frac{1}{2} \left| \int_{a_i}^{b_i} f''(t)(x-x_i)^2 dx \right| \\ &\le \frac{1}{2} \max_{t\in[a_i,b_i]} |f''(t)| \left| \underline{\int_{a_i}^{b_i} (x-x_i)^2 dx} \right| \\ &= \frac{h^3}{24} \max_{t\in[a_i,b_i]} |f''(t)| . \end{aligned}$$

$$\begin{aligned} \int_{a_i}^{b_i} (x-x_i)^2 dx &= \left[\frac{1}{3}(x-x_i)^3 \right]_{a_i}^{b_i} \\ &= \frac{1}{3}\left(\frac{h}{2}\right)^3 - \frac{1}{3}\left(-\frac{h}{2}\right)^3 \\ &= \frac{h^3}{12} \end{aligned}$$

$\|f''\|_\infty := \max_{t\in[a,b]} |f''(t)|$

Therefore,

$$|E| \le \frac{h^3}{24} \underbrace{\sum_{i=0}^{n-1} \max_{t\in[a_i,b_i]} |f''(t)|}_{\le \|f''\|_\infty} \le \frac{\cancel{h^3}}{24} \cancel{n} \overset{=b-a}{} \|f''\|_\infty = \underline{\frac{h^{\boxed{2}}}{24} \|f''\|_\infty (b-a)}, \rightarrow O(h^2)$$

where $hn = b - a$.

$n \cdot h = b - a$

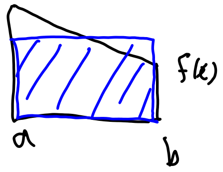
$h = \frac{b-a}{n}$

Error bounds for several cases

- Rectangular rule $\rightarrow \frac{h^{\boxed{2}}}{24}(b-a)\|f''\|_\infty$ if $f(x)$ is linear (or less) then exact

$\wedge$

- Trapezoidal rule $\rightarrow \frac{h^{\boxed{2}}}{12}(b-a)\|f''\|_\infty$ if $f(x)$ is linear (or less) then exact



- Simpson rule $\rightarrow \frac{h^4}{2880}(b-a)\|f''''\|_\infty$ if $f(x)$ is 3rd-order (or less) then exact

$$\int_{a_i = x_0}^{b_i = x_2} f(x)dx \sim [f(a_i) + 4f(c_i) + f(b_i)] \frac{h}{3}$$

next lecture

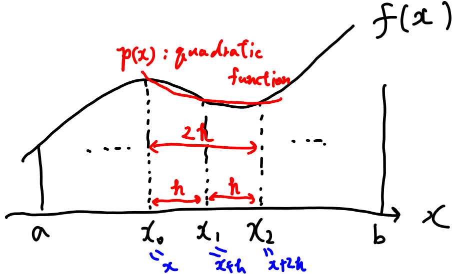
4 Simpson's rule (Quadratic interpolation)

x^2

Simpson's rule is a numerical integration formula based on quadratic interpolations. That is, for a target function $f \in C([a,b])$, we consider a quadratic interpolation in the form

$$p(x) = \alpha x^2 + \beta x + \gamma,$$

where $\alpha, \beta, \gamma \in \mathbb{R}$.



We can determine α, β, γ by solving

$$\begin{cases} \alpha x_0^2 + \beta x_0 + \gamma = f(x_0), \\ \alpha x_1^2 + \beta x_1 + \gamma = f(x_1), \\ \alpha x_2^2 + \beta x_2 + \gamma = f(x_2), \end{cases}$$

then compute $\int_{x_0}^{x_2} p(x)dx$ as an approximation for $\int_{x_0}^{x_2} f(x)dx$.

General expression

Solving the above system is tedious in general. To determine α, β, γ more efficiently, we consider the following general expression with the the three quadratic functions L_0, L_1, L_2 satisfying,

$$\begin{cases} L_0(x_0) = 1, & L_0(x_1) = L_0(x_2) = 0, \\ L_1(x_1) = 1, & L_1(x_2) = L_1(x_0) = 0, \\ L_2(x_2) = 1, & L_2(x_0) = L_2(x_1) = 0. \end{cases}$$

Using these functions, we have

$$p(x) = f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x)$$

In particular, these can be characterized as

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}, \quad L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}.$$

By integrating them from x_0 to x_2 under the condition $x_2 - x_1 = x_1 - x_0 = h$, we have

$$\int_{x_0}^{x_2} L_0(x)dx = \frac{h}{3}, \quad \int_{x_0}^{x_2} L_1(x)dx = \frac{4}{3}h, \quad \int_{x_0}^{x_2} L_2(x)dx = \frac{h}{3}.$$

Therefore, we have

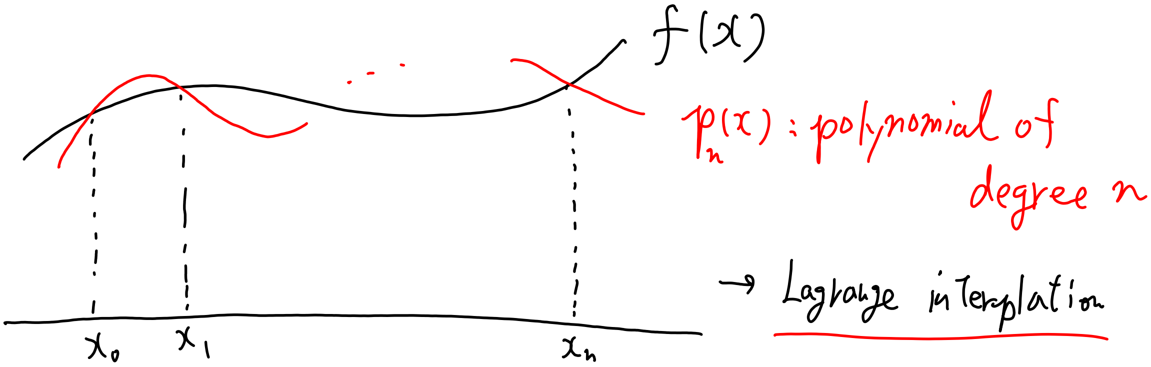
$$\int_{x_0}^{x_2} p(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

In fact, it is known that

$$\left| \int_a^b f(x)dx - \int_a^b p(x)dx \right| \le C(b-a)h^4 \|f''''\|_\infty$$

5 Lagrange interpolation (a generalization of Simpson's rule)

In the previous section, we learned Simpson's rule, a formula based on **quadratic** interpolation. Is it possible to create formulas based on higher order interpolation? The answer is yes.



We first define

$$L_k(x) := \prod_{\substack{j=0 \\ j\neq k}}^{n} \frac{x - x_j}{x_k - x_j} \quad (k = 0, 1, \cdots, n).$$

They satisfy

$$L_k(x_j) = \begin{cases} 1 & (j = k) \\ 0 & (j \neq k) \end{cases} \quad (j = 0, 1, \cdots, n).$$

Using these, the Lagrange interpolation $p_n(x)$ of degree n is written by

$$p_n(x) = \sum_{j=0}^{n} f(x_j) L_j(x).$$

The formula with similar intervals $a = x_0, x_1 = x_0 + h, x_2 = x_1 + h, \cdots, x_n = b$ is called the **Newton–Cotes rule**, which can be written in

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

where

$$\alpha_i := \int_a^b L_i(x)dx = (-1)^{n-i} \frac{h}{n!} \binom{n}{i} \int_0^n \frac{t(t-1)\cdots(t-n)}{t-i} dt$$

In fact, unfortunately, high degree Newton–Cotes rules are NOT effective.
*Find out about Runge's phenomenon.

200 ~ 500 words or more

6 Hermite interpolation

The Lagrange interpolation depends on the values of f on some sampling points. The Hermite interpolation is determined not only by such values but also by the values of derivative f'.

A polynomial $q_{2n+1}(x)$ of degree $2n+1$ satisfying

2n+2 eqations

$$\begin{cases} q_{2n+1}(x_j) = f(x_j) \\ q'_{2n+1}(x_j) = f'(x_j) \end{cases} \quad (j = 0, 1, \cdots, n)$$

is called the **Hermite interpolation polynomial**.

$$\begin{cases} H_k(x) & := L_k(x)^2[1 - 2L'_k(x_k)(x - x_k)] & \leftarrow 2n+1 \text{ degree} \\ K_k(x) & := L_k(x)^2(x - x_k) & \leftarrow 2n+1 \text{ degree} \end{cases}$$

Here, we have

$$\begin{cases} H_k(x_j) = \begin{cases} 1 & (j = k) \\ 0 & (j \neq k) \end{cases} & , \quad H'_k(x_j) = 0 \\ K_k(x_j) = 0 & , \quad K'_k(x_j) = \begin{cases} 1 & (j = k) \\ 0 & (j \neq k) \end{cases} \end{cases},$$

The Hermite interpolation polynomial is designed by

$$q_{2n+1}(x) = \sum_{j=0}^{n} \left[f(x_j)H_j(x) + f'(x_j)K_j(x) \right].$$

Using this, we have a integration formula

$$\int_a^b q_{2n+1}(x)dx = \sum_{i=0}^{n} \left[\alpha_i f(x_i) + \cancel{\beta_i f'(x_i)} \right],$$

where

$$\alpha_i = \int_a^b H_i(x)dx, \quad \beta_i = \int_a^b K_i(x)dx.$$

Note that we can choose the points $x_0, x_1, \cdots, x_n$ so that

$$\beta_i = 0 \text{ for all } i = 0, 1, \cdot, n.$$

This is really helpful to implement numerical integrations. We will learn the choice ~~from~~ in the next section and obtain very accurate integration formulas.

6.1 Inner product

For a (real) vector space V, the map $(\cdot,\cdot) : V \times V \to \mathbb{R}$ that satisfies the following is called **inner product**:

Inner product

1. $(x,x) \geq 0, \ ^{\forall}x \in V$, in particular $(x,x) = 0 \Longleftrightarrow x = 0$
2. $(x,y) = (y,x), \ ^{\forall}x, y \in V$
3. $$\begin{aligned}(ax+by,z) &= a(x,z)+b(y,z)\\ (x,ay+bz) &= a(x,y)+b(x,z)\end{aligned} \qquad ^{\forall}x,y,z \in V, \ ^{\forall}a,b \in V$$

Vectors x and y are called orthogonal when

$$(x,y) = 0, \quad x \neq 0, \ y \neq 0,$$

which is denoted by $x \perp y$. Hereafter, we endow $V = C([a,b])$ (the set of continuous functions over $[a,b]$) with the inner product

$$(p,q)_w = \int_a^b p(x)q(x)w(x)dx, \quad p,q \in V,$$

where $w \in V$ is called the weight function that satisfies

1. $w(x) > 0, \quad a < x < b$ (Positivity),
2. $\int_a^b w(x)dx < \infty$ (Integrable).

6.2 Orthogonal polynomial system

Orthogonal polynomial system over $[a,b] \subset \mathbb{R}$ with respect to a weight function w is the set

$$\{\phi_0, \phi_1, \cdots, \phi_n\} \subset C([a,b])$$

such that

1. ϕ_0 : (nonzero) constant function, for example, $\phi_0(x) = 1$,
2. ϕ_k : polynomial with k degree with $1 \leq k \leq n$,
3. $\phi_i \perp \phi_j \ (i \neq j)$ with respect to w, that is, $(\phi_i, \phi_j)_w = 0 \ (i \neq j)$.

6.2.1 Famous orthogonal polynomials

Example 1) Chebyshev polynomials

The polynomials over $[-1,1]$ defined by

$$\begin{aligned}T_0(x) &= 1\\ T_1(x) &= x\\ T_{i+1}(x) &= 2xT_i(x) - T_{i-1}(x), \quad i = 1,2,\cdots\end{aligned}$$

are called the **Chebyshev polynomials**. These satisfy

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

for the weight function $\boxed{w(x) = \dfrac{1}{\sqrt{1-x^2}}}$

Example 2) Legendre polynomials

The polynomials over $[-1, 1]$ defined by

$$\begin{aligned} &P_0(x) = 1 \\ &P_i(x) = \frac{1}{2^i i!}\frac{d^i}{dx^i}(x^2-1)^i, \quad i = 1, 2, \cdots \\ &(P_i, P_j)_{\boxed{w(=1)}} = \int_{-1}^{1} P_i(x)P_j(x)dx = \begin{cases} 0 \quad (i \neq j) \\ \frac{2}{2i+1} \quad (i = j) \end{cases} \end{aligned}$$

are called **Legendre polynomials**.

6.3 Gaussian quadrature

The following is known for a system of orthogonal polynomials:

Theorem 6.1

For a system of orthogonal polynomials $\{\phi_0, \phi_1, \cdots, \phi_n\}$ with respect to weight w, we have

(i) Arbitrary polynomials q_n with degree n are written in the linear combination:

$$q_n = a_0\phi_0 + a_1\phi_1 + \cdots + a_n\phi_n, \quad a_i \in \mathbb{R}.$$

(ii) Let $k < n$. For a polynomial q_k with degree k,

$q_k = a_0 \underline{\phi_0} + \cdots + a_k \underline{\phi_k}$

$$(\underline{\underline{\phi_n}}, q_k)_w = 0.$$

(iii) $\phi_n(x)$ have n different zeros (solution of $\phi_n(x) = 0$).

We consider the approximation

$$\int_a^b f(x)w(x)dx \sim \int_a^b \underline{q_{2n+1}(x)}w(x)dx.$$

based on the Hermite interpolation (see Section 6). Note that, ~~ff~~ if one needs $\int_a^b f(x)dx$, replace $f(x) \to f(x)/w(x)$. Then, we have the following integration formula

$$\int_a^b q_{2n+1}(x)w(x)dx = \sum_{i=0}^{n} [W_i f(x_i) + V_i f'(x_i)],$$

where $\overset{\alpha_i}{W_i = \int_a^b H_i(x)w(x)dx}$ and $\overset{\beta_i}{V_i} = \int_a^b K_i(x)w(x)dx$.

How do we choose x_i so that $V_i = 0$?

The answer is the following:

Theorem 6.2

Let $\{\phi_0, \phi_1, \cdots, \underline{\phi_{n+1}}\}$ be an orthogonal polynomial system with respect to $\underline{(\cdot,\cdot)_w}$. Moreover, we set

$$(a <)x_0 < x_1 < \cdots < x_n(< b) \text{ as } \underline{\text{the zeros of } \phi_{n+1}(x)}.$$

Then, $V_i = 0$ for all $\underline{i = 0, 1, 2, \cdots, n}$

Proof. ϕ_{n+1} can be written as

$$\phi_{n+1}(x) = \lambda(x - x_0)(x - x_1)\cdots(x - x_n)$$

with some $\lambda \in \mathbb{R}$. Therefore, this is further expressed as

$$\phi_{n+1}(x) = CL_i(x)\underline{(x - x_i)}$$

with some constant $C \in \mathbb{R}$, where recall that

$$L_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}$$

Therefore, it follows that

$$\begin{aligned} V_i &= \int_a^b L_i(x)^2(x - x_i)w(x)dx \\ &= \int_a^b \underbrace{L_i(x)(x - x_i)}_{= \phi_{n+1}/C} L_i(x)w(x)dx \\ &= \frac{1}{C}\int_a^b \phi_{n+1}(x)\underset{/\!/}{L_i(x)}w(x)dx \\ &= \frac{1}{C}(\underset{i \leq n}{L_i(x)}, \phi_{n+1})_w = 0 \end{aligned}$$

because the degree of L_i is n. □

A simple calculation leads to

$$W_i = \int_a^b L_i(x)^2(x)w(x)dx \ (> 0).$$

$$\|$$

In fact, we have

$$\boxed{W_i = \int_a^b L_i(x)w(x)dx}$$

Indeed, for $g_k(x) = (x - x_0)(x - x_1) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)$ (of degree n), we have

$$\int_a^b g_k(x)w(x)dx = \sum_{i=0}^{n} W_i g_k(x_i) = W_k g(x_k)$$

Therefore,

$$W_k = g(x_k)^{-1} \int_a^b g_k(x)w(x) = \int_a^b L_i(x)w(x)dx.$$

Summarizing the above-mentioned discussion, we have the following integration formula, called the **Gaussian quadrature**: $\int_a^b f(x)w(x)dx$

$\wr$

$$\begin{cases} \displaystyle\int_a^b q_{2n+1}(x)w(x)dx = \sum_{i=0}^{n} W_i f(x_i) \\ \displaystyle\underset{d_i}{W_i} = \int_a^b L_i(x)w(x)dx. \end{cases}$$

Note that this gives the exact integration for $f(x)$ with degree $\leq 2n + 1$.

Theorem 6.3

Given $f \in C([a, b])$,

$$\lim_{n\to\infty} \sum_{i=0}^{n} W_i f(x_i) = \int_a^b f(x)w(x)dx.$$

6.3.1 Gauss-Chebyshev quadrature

$x \in [-1, 1]$

$x = 2y - 1$

$\Leftrightarrow y = \frac{x+1}{2} \in [0, 1]$

$\int_0^1 y^2 dy$

$= \int_{-1}^1 \left(\frac{x+1}{2}\right)^2 \cdot \frac{dx}{2}$

Let $[a, b] = [-1, 1]$, $\quad w(x) = \dfrac{1}{\sqrt{1 - x^2}}$.

$$\int_a^b f(x)w(x)dx \sim \sum_{i=0}^{n} W_i f(x_i),$$

$$\int_{-1}^{1} (1 - x^2)^{\frac{3}{2}} dx$$

$$= \int_{-1}^{1} \underbrace{(1 - x^2)^2}_{f(x)} \underbrace{\frac{1}{\sqrt{1 - x^2}}}_{w(x)} dx$$

where

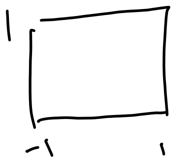
$\phi_{n+1}(x_i) = 0$

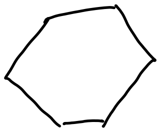
$$x_i = \cos\frac{(i + \frac{1}{2})\pi}{n + 1}, \quad W_i = \frac{\pi}{n + 1} \quad (i = 0, 1, 2, \cdots, n)$$

6.3.2 Gauss-Legendre quadrature

Let $[a, b] = [-1, 1]$, $\quad w(x) = 1$.

$$\int_a^b f(x) \cdot 1 dx \sim \sum_{i=0}^{n} W_i f(x_i),$$





where x_i are zeros of the Legendre polynomial $P_{n+1}(x)$, and

$$W_i = \int_a^b L_i(x)dx$$

.