# 計算固体力学入門 (2)

## Introduction to Computational Solid Mechanics (2)

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# Today's topic

The contents of this course will be as follows:

1. FEM for a one-dimensional problem.

2. Mathematical preliminaries
   - **Gauss-Legendre quadrature**
   - Einstein's summation convention

3. Continuum mechanics
   - Deformation of continuum
   - Balance of continuum
   - Basic equations

**mid-term**

4. Weak form

5. Discretization

6. FEM implementations

**final**

# Introduction

In the previous lecture, we have studied the very basics of FEM.
In the FEM, the solution $u(x)$ of a BVP is approximated as

$$\tilde{u}(x) = \sum_{i=0}^{n-1} a_i g_i(x),$$

with the unknown coefficients $a_i$ and basis functions $g_i(x)$. The unknown coefficients are determined by the following algebraic equations:

$$\sum_{j=0}^{n-1} \left( \int_0^1 g_i'(x) g_j'(x) \mathrm{d}x \right) a_j = \int_0^1 g_i f(x) \mathrm{d}x,$$

derived from the weighted residual equation, the weak form, and the Galerkin discretization.

**ISSUE:** How can we compute the integrals?

➡ **Numerical integration (quadrature)**

# What is quadrature?

For example, let us consider a given definite integral such as

$$I = \int_a^b f(x)\mathrm{d}x\,. \qquad (1)$$

The **quadrature rule** for (1) is generally written as

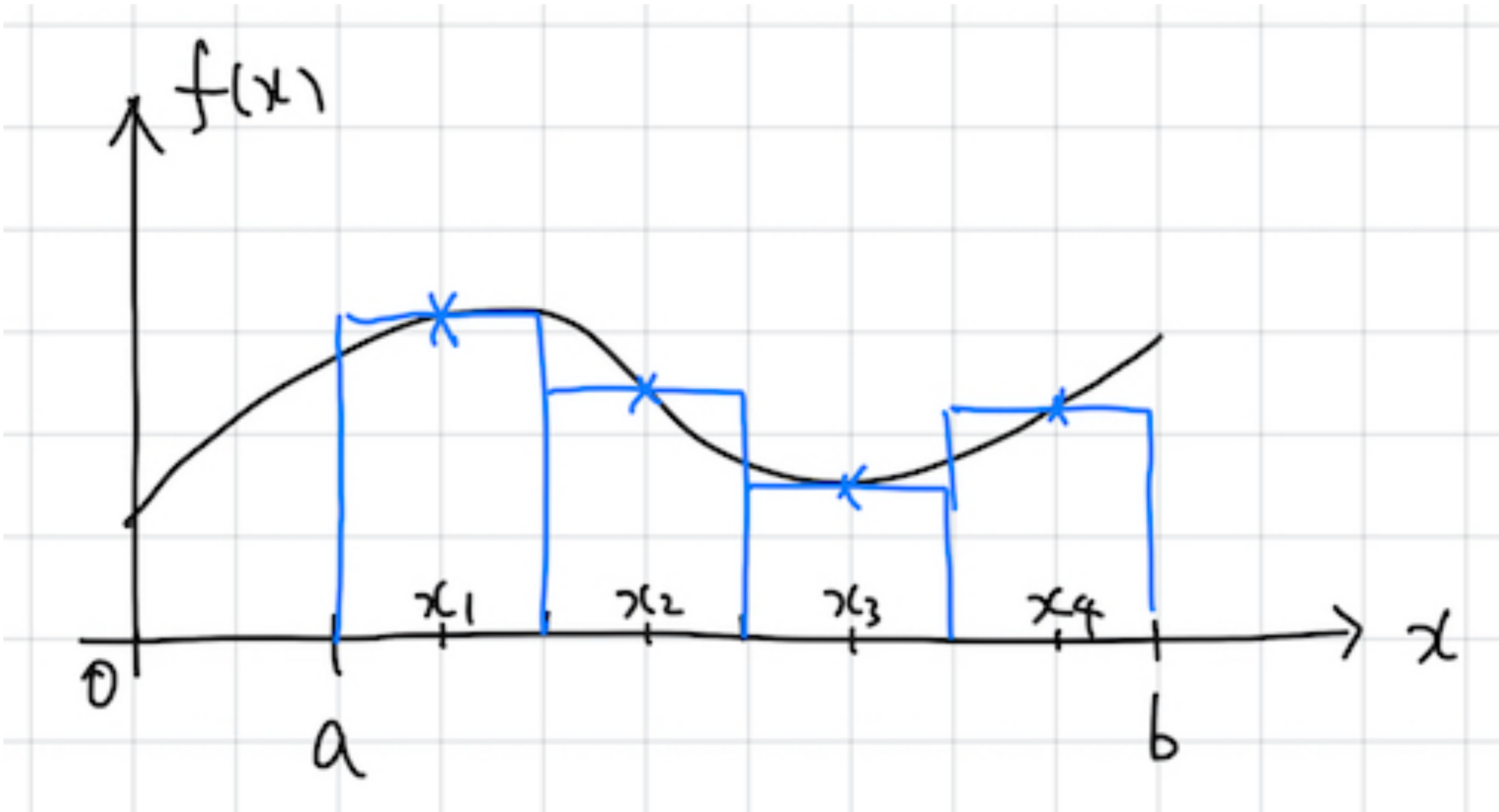
$$I \simeq \sum_{i=1}^{N} f(x_i)w_i, \qquad (2)$$

where $x_i \in [a, b]$ and $w_i > 0$ are the integral point and weight, respectively. The rule with $N$ integral points is referred as quadrature of degree $N$.

**NOTE:** (2) is much easier than (1) to compute,
and involves only addition and multiplication.

# Famous examples 1/2

The simplest quadrature rule is the quadrature by parts (or sectional quadrature).

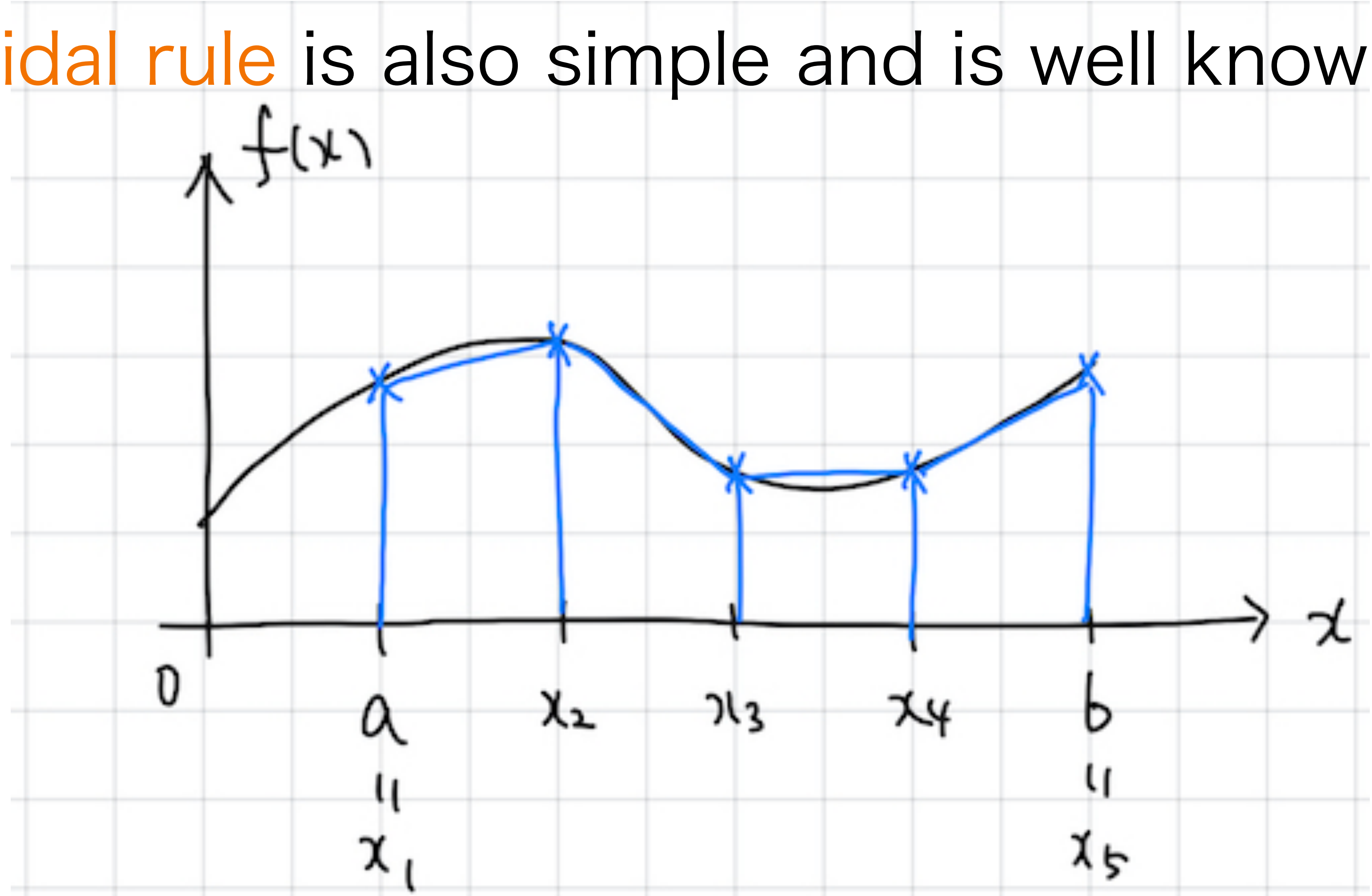



- The range $[a, b]$ is divided into $N$ sections of equal length.
- The integral points and weights are respectively chosen as

$$x_i = a + \frac{2i-1}{2N}(b-a), \quad w_i = \frac{b-a}{N}.$$

# Famous examples 2/2

The trapezoidal rule is also simple and is well known.




- The range $[a, b]$ is divided into $N-1$ sections of equal length.
- The integral points and weights are respectively chosen as

$$x_i = a + \frac{i-1}{N}(b-a),$$

$$w_1 = w_N = \frac{b-a}{2N}, w_2 = w_3 = \cdots = w_{N-1} = \frac{b-a}{N}.$$

# Simple question

It seems that the trapezoidal rule is more accurate than the sectional quadrature. The trapezoidal rule, however, can be exact only when the integrand is (piecewise) linear function.

→ Can we design a quadrature rule which can compute

$$I = \int_a^b f(x)\mathrm{d}x, \quad (1)$$

exactly (=without error) for functions $f$ in a certain class?

**Gauss-Legendre (GL) quadrature**

$N^{\mathrm{th}}$-order GL rule can compute (1) exactly when $f$ is a polynomial of at most of order $2N-1$.

# Preliminaries

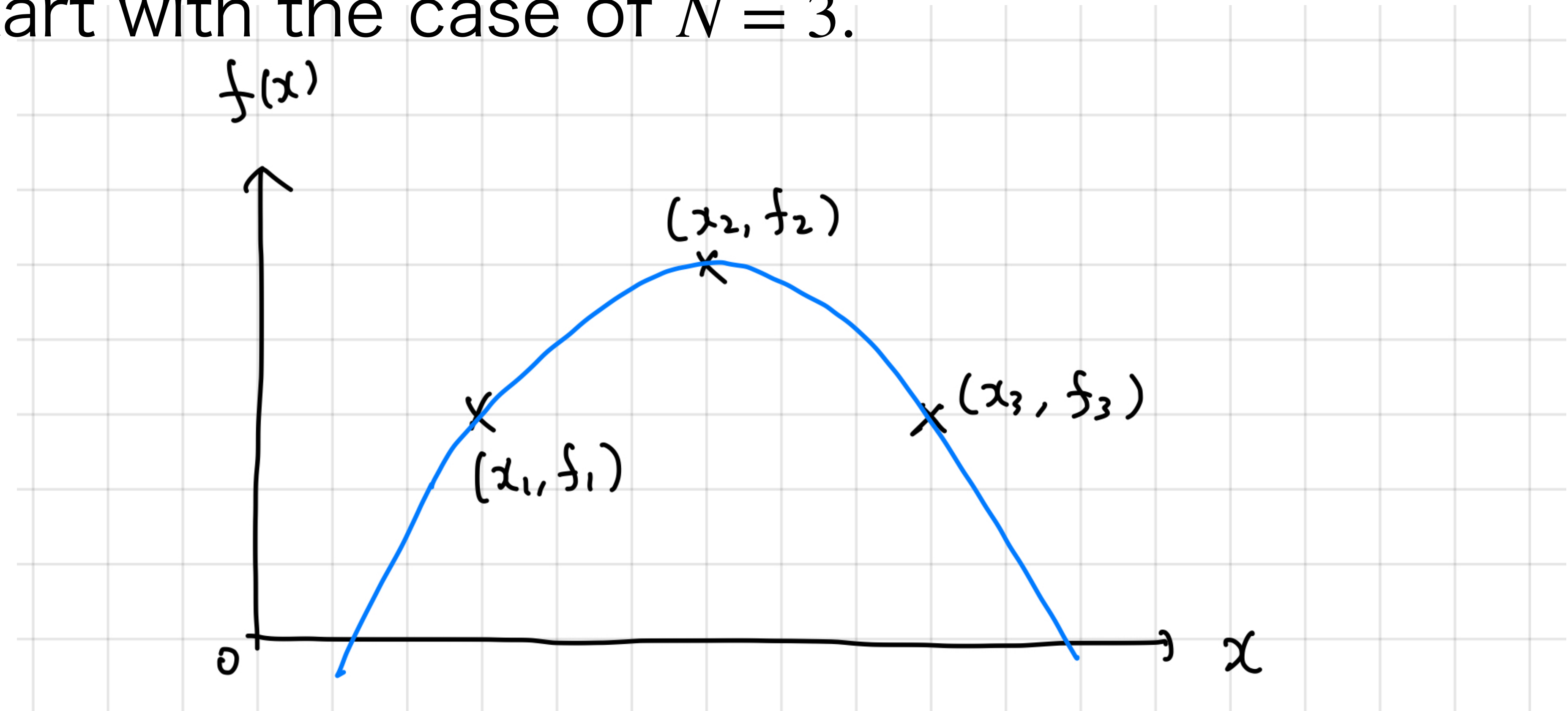
To derive the GL quadrature, let us introduce the following tools:

- Legendre interpolation
- Legendre polynomial

# Legendre interpolation 1/3

Let us find a polynomial of degree $N$ such that $f(x_i) = f_i$ for a given set of data $(x_1, f_1), \cdots, (x_N, f_N)$.

Let us start with the case of $N = 3$.




By letting $f$ as $f(x) = ax^2 + bx + c$, with the unknown coefficients $a, b, c$, we can easily find the Legendre interpolation by solving

$$f_i = ax_i^2 + bx_i + c$$

for $a, b, c$, but...

# Legendre interpolation 2/3

Since such a polynomial is unique, we can easily see $f$ can be written as

$$f(x) = \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)} f_1 + \frac{(x - x_3)(x - x_1)}{(x_2 - x_3)(x_2 - x_1)} f_2 + \frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)} f_3$$

**Quiz 1.**

Find the linear function passing through $(x_1, f_1)$ & $(x_2, f_2)$.

# Legendre interpolation 3/3

**Legendre interpolation of degree $N$**

$$f(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} f_1 + \frac{(x-x_3)(x-x_1)}{(x_2-x_3)(x_2-x_1)} f_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} f_3$$

$\downarrow$ generalise

**Legendre interpolation of degree $N$**

$$f(x) = \sum_{i=1}^{N} \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} f_i \qquad (4)$$

# Legendre polynomial 1/3

## Legendre polynomial $p_n(x)$ (of degree $n$)

(one of the) so called **orthogonal polynomials**

**definition:** a polynomial $p_n(x)$ satisfying

$$\int_{-1}^{1} p_n(x)p_k(x)\mathrm{d}x = 0\ , \qquad (5)$$

for $k = 0,\cdots,n-1$.

- Why do we call this orthogonal?

  → Because $\int_{-1}^{1} f(x)g(x)\mathrm{d}x$ is the inner product.

- $p_n(x)$ is uniquely determined by (5) up to constant factor.

  → We here normalise it such that $p_n(1) = 1$, (6)

Note: This normalisation does not give an orthonormal system, and the way of normalisation is different from author by author.

# Legendre polynomial 2/3

**Quiz 2.**

Give the explicit representation of $p_0(x), p_1(x), p_2(x)$

# Legendre polynomial 3/3

**Properties of the Legendre polynomials:**

- (Rodrigues' formula)

$$p_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left[(x^2-1)^n\right] \tag{7}$$

- (Bonnet's recursion formula)

$$(n+1)p_{n+1}(x) = (2n+1)xp_n(x) - np_{n-1}(x) \tag{8}$$

- For any polynomial $q_k(x)$ of order $k$ $(\leq n-1)$, we have

$$\int_{-1}^{1} p_n(x)q_k(x)\mathrm{d}x = 0. \tag{9}$$

# The GL quadrature 1/10

Let us now derive the Gauss-Legendre quadrature rule. To begin with, we consider the following definite integral:

$$I = \int_{-1}^{1} f_3(x)\mathrm{d}x,$$

where $f_3$ is a third order polynomial.

First, we “divide” $f_3$ by $p_2$ to have

$$f_3(x) = p_2(x)q_1(x) + r_1(x), \tag{10}$$

where $q_1$ and $r_1$ are first order polynomials. Then,

$$\begin{aligned} I &= \int_{-1}^{1} f_3(x)\mathrm{d}x \\ &= \int_{-1}^{1} p_2(x)q_1(x)\mathrm{d}x + \int_{-1}^{1} r_1(x)\mathrm{d}x \\ &= \int_{-1}^{1} r_1(x)\mathrm{d}x \end{aligned} \tag{11}$$

# The GL quadrature 2/10

We then rewrite $r_1(x)$ by the Lagrange interpolation with the "data"$(x_1, r_1(x_1))$ & $(x_2, r_1(x_2))$ to see

$$
\begin{aligned}
I &= \int_{-1}^{1} r_1(x)\mathrm{d}x \\
&= \int_{-1}^{1} \frac{x - x_2}{x_1 - x_2} r_1(x_1)\mathrm{d}x + \int_{-1}^{1} \frac{x - x_1}{x_2 - x_1} r_1(x_2)\mathrm{d}x \\
&= \frac{-2x_2}{x_1 - x_2} r_1(x_1) + \frac{-2x_1}{x_2 - x_1} r_1(x_2)\,. \qquad (12)
\end{aligned}
$$

Since $x_1$ and $x_2$ are arbitrary, let us choose the "zeros" of $p_2(x)$, i.e. $p_2(x_i) = 0$ so that, recalling (10), we have

$$
f_3(x_i) = r_1(x_i)\,. \qquad (13)
$$

# The GL quadrature 3/10

By substituting (13) into (12), we have

$$I = \frac{-2x_2}{x_1 - x_2} f(x_1) + \frac{-2x_1}{x_2 - x_1} f(x_2), \tag{14}$$

which can further be rewritten by exploiting the explicit formula for $p_2(x) = (3x^2 - 1)/2$ as follows:

$$I = \int_{-1}^{1} f_3(x)\mathrm{d}x = 1 \times f_3(-1/\sqrt{3}) + 1 \times f_3(1/\sqrt{3}) \,. \tag{15}$$

(15) is nothing but the Gauss-Legendre quadrature of $N = 2^{\text{th}}$ degree, with $x_1 = -1/\sqrt{3}, x_2 = +1/\sqrt{3}, w_1 = w_2 = 1.$

**Note:** (15) is exact for all polynomials of at most third degree.

# The GL quadrature 4/10

the Gauss-Legendre quadrature of $N = 2^{\text{th}}$ degree: $x_1 = -1/\sqrt{3}, x_2 = +1/\sqrt{3}, w_1 = w_2 = 1.$

**(Quiz)** Compute the following definite integrals by second order GL quadrature:

$$(a) \quad \int_{-1}^{1} (x^2 + 3x + 1)\mathrm{d}x = \frac{8}{3} \simeq 2.6667$$

$$(b) \quad \int_{-1}^{1} (x^4 + 3x^3 + 2x^2 + x + 3)\mathrm{d}x = \frac{116}{15} \simeq 7.7333$$

# The GL quadrature 5/10

As indicated in the previous example, the 2nd order GL rule is exact when the integrand is 2nd order, while not when the integrand is 4th order. In general, $N$th order GL rule is exact when the integrand is up to 3rd order.

Note: $N$th order quadrature has the degrees of freedom of $2N$, i.e. $N$ integral points and $N$ weights, which is identical to the number of coefficients of a polynomial of $2N-1$ degree, i.e. the number of $\{a_i\}s$ for $a_0 + a_1 x + \cdots + a_{2N-1} x^{2N-1}$.

In this sense, the GL quadrature is an **optimal** rule. Note, however, that it does not necessary guarantee the accuracy for integrands

# The GL quadrature 6/10

Can we always have the integral points $x_i$ such that $-1 \leq x_i \leq 1$?
$\rightarrow$ Yes!

**Theorem**

The zeros of the Legendre polynomial of order $(n \geq 1)$ are all simple (i.e. all the zeros are distinct each other), and exist in $(-1, 1)$.

(proof)

# The GL quadrature 7/10

How to compute the zeros of $p_n(x)$?
$\rightarrow$ Golub-Welsch's algorithm.

According to Bonnet's recursion formula (8), we have

$$xp_n(x) = \frac{n}{2n+1} p_{n-1}(x) + \frac{n+1}{2n+1} p_{n+1}(x)$$

$$\Leftrightarrow x \begin{pmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{N-2}(x) \\ p_{N-1}(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \frac{1}{3} & 0 & \frac{2}{3} & \ddots & \vdots \\ 0 & \frac{2}{5} & 0 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \frac{n-1}{2n-3} \\ 0 & \cdots & 0 & \frac{n-1}{2n-1} & 0 \end{pmatrix} \begin{pmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{N-2}(x) \\ p_{N-1}(x) \end{pmatrix} + \begin{pmatrix} 0 \\ \vdots \\ \vdots \\ 0 \\ \frac{n}{2n-1} p_N(x) \end{pmatrix}$$

Let us substitute $x = x_j$ ($j$th zero of $p_N$, i.e. $p_N(x_j) = 0$) to have...

# The GL quadrature 8/10

How to compute the zeros of $p_n(x)$?
→ Golub-Welsch's algorithm.

$$x_j \begin{pmatrix} p_0(x_j) \\ p_1(x_j) \\ \vdots \\ p_{N-2}(x_j) \\ p_{N-1}(x_j) \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \frac{1}{3} & 0 & \frac{2}{3} & \ddots & \vdots \\ 0 & \frac{2}{5} & 0 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \frac{n-1}{2n-3} \\ 0 & \cdots & 0 & \frac{n-1}{2n-1} & 0 \end{pmatrix} \begin{pmatrix} p_0(x_j) \\ p_1(x_j) \\ \vdots \\ p_{N-2}(x_j) \\ p_{N-1}(x_j) \end{pmatrix}$$

which is an eigenvalue problem $x_j \boldsymbol{p} = \mathrm{A}\boldsymbol{p}$ (which can be solved numerically e.g. Lapack routines).

# The GL quadrature 9/10

Once we obtain the integral points $x_j$, we can compute the corresponding weights $w_j$ by using the fact that

$$\int_{-1}^{1} \prod_{i=1, i \neq j}^{N} (x - x_i)\mathrm{d}x = \sum_{i=1}^{N} f(x_i) w_i = f(x_j) w_j$$

holds exactly as

$$w_j = \frac{\int_{-1}^{1} \prod_{i=1, i \neq j}^{N} (x - x_i)\mathrm{d}x}{f(x_j)}$$

Note that the above integral can exactly be computed by, for example, the GL quadrature of $N/2$th degree.

Do you want to change the range of the integral? You can this as

$$\int_{a}^{b} f(x)\mathrm{d}x = \int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right)\mathrm{d}x$$

# The GL quadrature 10/10

## Summary

The GL quadrature compute

$$I = \int_a^b f(x)\mathrm{d}x \simeq \sum_{i=1}^{N} f(x_i)w_i,$$

and the result is exact when $f$ is a polynomial up to of order $2N-1$.

```
N=1
i   integral point                                        weight
1   0.000000000000000000000000000000000000        2.000000000000000000000000000000000000

N=2
i   integral point                                        weight
1 -0.577350269189625764509148780501957505        0.999999999999999999999999999999999904
2  0.577350269189625764509148780501957505        0.999999999999999999999999999999999904

N=3
i   integral point                                        weight
1 -0.774596669241483377035853079956479975        0.555555555555555555555555555555555384
2  5.64237288394698003824993537866677925E-0037    0.888888888888888888888888888888888268
3  0.774596669241483377035853079956480071        0.555555555555555555555555555555555384

N=4
i   integral point                                        weight
1 -0.861136311594052575223946488892809554        0.347854845137453857373063949221999619
2 -0.339981043584856264802665759103244761        0.652145154862546142626936050778000574
3  0.339981043584856264802665759103244712        0.652145154862546142626936050778000285
4  0.861136311594052575223946488892809457        0.347854845137453857373063949221999619

N=5
i   integral point                                        weight
1 -0.906179845938663992797626878299392925        0.236926885056189087514264040719917379
2 -0.538469310105683091036314420700208927        0.478628670499366468041291514835638128
3   3.54466792529882068759881776526999728E-0035   0.568888888888888888888888888888889081
4  0.538469310105683091036314420700208831        0.478628670499366468041291514835637839
5  0.906179845938663992797626878299392828        0.236926885056189087514264040719917644
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