Theoretical foundations of Gaussian quadrature

1 Inner product vector space

Definition 1. *A* vector space *(or* linear space*) is a set* $V = \{\mathbf{u}, \mathbf{v}, \mathbf{w}, \ldots\}$ *in which the following two operations are defined:*

(A) Addition of vectors: $\mathbf{u} + \mathbf{v} \in V$*, which satisfies the properties*

- *(A₁) associativity:* $\mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w} \quad \forall$ $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$ *in* V*;*
- *(A₂) existence of a zero vector:* $\exists\ \mathbf{0} \in V$ *such that* $\mathbf{u} + \mathbf{0} = \mathbf{u} \quad \forall \mathbf{u} \in V$*;*
- *(A₃) existence of an opposite element:* $\forall \mathbf{u} \in V\ \exists (-\mathbf{u}) \in V$ *such that* $\mathbf{u} + (-\mathbf{u}) = \mathbf{0}$*;*
- *(A₄) commutativity:* $\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u} \quad \forall$ $\mathbf{u}$, $\mathbf{v}$ *in* V*;*

(B) Multiplication of a number and a vector: $\alpha \mathbf{u} \in V$ *for* $\alpha \in \mathbb{R}$*, which satisfies the properties*

- *(B₁)* $\alpha(\mathbf{u} + \mathbf{v}) = \alpha \mathbf{u} + \alpha \mathbf{v} \quad \forall\ \alpha \in \mathbb{R}, \forall \mathbf{u}, \mathbf{v} \in V$*;*
- *(B₂)* $(\alpha + \beta)\mathbf{u} = \alpha \mathbf{u} + \beta \mathbf{u} \quad \forall\ \alpha, \beta \in \mathbb{R}, \forall \mathbf{u} \in V$*;*
- *(B₃)* $(\alpha\beta)\mathbf{u} = \alpha(\beta \mathbf{u}) \quad \forall\ \alpha, \beta \in \mathbb{R}, \forall \mathbf{u} \in V$*;*
- *(B₄)* $1\mathbf{u} = \mathbf{u} \quad \forall \mathbf{u} \in V$*.*

Definition 2. *An* inner product linear space *is a linear space* V *with an operation* $(\cdot, \cdot)$ *satisfying the properties*

- *(a)* $(\mathbf{u}, \mathbf{v}) = (\mathbf{v}, \mathbf{u}) \quad \forall$ $\mathbf{u}$, $\mathbf{v}$ *in* V*;*
- *(b)* $(\mathbf{u} + \mathbf{v}, \mathbf{w}) = (\mathbf{u}, \mathbf{w}) + (\mathbf{v}, \mathbf{w}) \quad \forall$ $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$ *in* V*;*
- *(c)* $(\alpha \mathbf{u}, \mathbf{v}) = \alpha(\mathbf{u}, \mathbf{v}) \quad \forall \alpha \in \mathbb{R}, \forall$ $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$ *in* V*;*
- *(d)* $(\mathbf{u}, \mathbf{u}) \geq 0 \quad \forall \mathbf{u} \in V$*; moreover,* $(\mathbf{u}, \mathbf{u}) = 0$ *if and only if* $\mathbf{u} = \mathbf{0}$.

Example. The "standard" inner product of the vectors $\mathbf{u} = (u_1, u_2, \ldots, u_d) \in \mathbb{R}^d$ and $\mathbf{v} = (v_1, v_2, \ldots, v_d) \in \mathbb{R}^d$ is given by

$$(\mathbf{u}, \mathbf{v}) = \sum_{i=1}^{d} u_i v_i\ .$$

Example. Let $\mathbf{G}$ be a symmetric positive-definite matrix, for example

$$\mathbf{G} = (g_{ij}) = \begin{pmatrix} 5 & 4 & 1 \\ 4 & 7 & 0 \\ 1 & 0 & 3 \end{pmatrix} .$$

Then one can define a scalar product corresponding to $\mathbf{G}$ by

$$(\mathbf{u}, \mathbf{v}) := \sum_{i=1}^{d} \sum_{j=1}^{d} u_i \, g_{ij} \, v_j \ .$$

Remark. In an inner product linear space, one can define the *norm* of a vector by

$$\|\mathbf{u}\| := \sqrt{(\mathbf{u}, \mathbf{u})} \ .$$

The famous *Cauchy-Schwarz inequality* reads

$$|(\mathbf{u}, \mathbf{v})| \le \|\mathbf{u}\| \, \|\mathbf{v}\| \ .$$

Think about the meaning of this inequality in $\mathbf{R}^3$.

Exercise. Find the norm of the vector $\mathbf{u} = (3, 0, -4)$ using the "standard" inner product in $\mathbf{R}^3$ and then by using the inner product in $\mathbf{R}^3$ defined through the matrix $\mathbf{G}$.

A very important example. Consider the set of all polynomials of degree no greater than 4, where the operations "addition of vectors" and "multiplication of a number and a vector" are defined in the standard way, namely: if P and Q are such polynomials,

$$P(x) = p_4 x^4 + p_3 x^3 + p_2 x^2 + p_1 x + p_0 \ , \qquad Q(x) = q_4 x^4 + q_3 x^3 + q_2 x^2 + q_1 x + q_0 \ ,$$

then their sum, $P + Q$ is given by

$$(P+Q)(x) = (p_4 + q_4) x^4 + (p_3 + q_3) x^3 + (p_2 + q_2) x^2 + (p_1 + q_1) x + (p_0 + q_0) \ ,$$

and, for $\alpha \in \mathbb{R}$, the product αP is defined by

$$(\alpha P)(x) = (\alpha p_4) x^4 + (\alpha p_3) x^3 + (\alpha p_2) x^2 + (\alpha p_1) x + (\alpha p_0) \ .$$

Then this set of polynomials is a vector space of dimension 5. One can take for a basis in this space the set of polynomials

$$E_0(x) := 1 \ , \quad E_1(x) := x \ , \quad E_2(x) := x^2 \ , \quad E_3(x) := x^3 \ , \quad E_4(x) := x^4 \ .$$

This, however, is only one of the infinitely many bases in this space. For example, the set of vectors

$$G_0(x) := x - 1 \ , \quad G_1(x) := x + 1 \ , \quad G_2(x) := x^2 + 3x + 3 \ ,$$

$$G_3(x) := -x^3 + 3x^2 - 4 \ , \quad G_4(x) := x^4 - x^3 - 2x$$

is a perfectly good basis. (Note that I called G_0, G_1, …, G_n "vectors" to emphasize that what is important for us is the structure of vector space and not so much the fact that these "vectors" are polynomials.) Any vector (i.e., polynomial of degree ≤ 4) can be represented in a unique way in any basis, for example, the polynomial $P(x) = 3x^4 - 5x^2 + x + 7$ can be written as

$$P = 3\,E_4 - 5\,E_2 + E_1 + 7\,E_0 \ ,$$

or, alternatively, as

$$P = 3\,G_4 - 3\,G_3 + 4\,G_2 - 11\,G_1 + 6\,G_0 \ .$$

2 Inner product in the space of polynomials

One can define an inner product structure in the space of polynomials in many different ways. Let $V_n(a,b)$ stand for the space of polynomials of degree $\le n$ defined for $x \in [a,b]$. Most of the theory we will develop works also if $a = -\infty$ and/or $b = \infty$. Let $w : [a,b] \to \mathbb{R}$ be a *weight function*, i.e., a function satisfying the following properties:

(a) the integral $\int_a^b w(x)\,\mathrm{d}x$ exists;

(b) $w(x) \ge 0$ for all $x \in [a,b]$, and $w(x)$ can be zero only at isolated points in $[a,b]$ (in particular, $w(x)$ cannot be zero in an interval of nonzero length).

We define a scalar product in $V_n(a,b)$ by

$$(P,Q) := \int_a^b P(x)\,Q(x)\,w(x)\,\mathrm{d}x \ ; \tag{1}$$

if the interval (a,b) is of infinite length, then one has to take w such that this integral exists for all P and Q in $V_n(a,b)$. Let $V_n(a,b;w)$ stands for the inner product linear space of polynomials of degree $\le n$ defined on $[a,b]$, and scalar product defined by (1).

Example. The *Legendre polynomials* are a family of polynomials P_0, P_1, P_2, … such that P_n is a polynomial of degree n defined for $x \in [-1,1]$, with leading coefficients equal to 1 ("leading" are the coefficients of the highest powers of x) and such that P_n and P_m are orthogonal for $n \ne m$ in the sense of the following inner product:

$$(P_n, P_m) = \int_{-1}^{1} P_n(x)\,P_m(x)\,\mathrm{d}x \ .$$

In other words, the polynomials P_0, P_1, P_2, …, P_n constitute an orthogonal basis of the space $V_n(-1,1;w(x)\equiv 1)$. Here are the first several Legendre polynomials:

$$P_0(x) = 1 \ , \quad P_1(x) = x \ , \quad P_2(x) = x^2 - \frac{1}{3} \ , \quad P_3(x) = x^3 - \frac{3}{5}x \ , \quad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35} \ , \ldots \ .$$

Sometime Legendre polynomials are normalized in a different way:

$$\tilde{P}_0(x) = 1 \ , \quad \tilde{P}_1(x) = x \ , \quad \tilde{P}_2(x) = \frac{1}{2}(3x^2 - 1) \ ,$$

$$\tilde{P}_3(x) = \frac{1}{2}(5x^3 - 3x) \ , \quad \tilde{P}_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3) \ , \dots \ ;$$

check that P_n is proportional to $\tilde{P}_n$ for all the polynomials given here.

Exercise. Check that each of the first five Legendre polynomials is orthogonal to all other Legendre polynomials in the example above.

Example. The *Hermite polynomials* are a family of polynomials H_0, H_1, H_2, $\dots$ such that H_n is a polynomial of degree n defined for $x \in \mathbb{R}$, normalized in such a way that $(H_n, H_n) = 2^n n! \sqrt{\pi}$ and $(H_n, H_m) = 0$ for $n \neq m$, where the inner product is defined as follows:

$$(H_n, H_m) = \int_{-\infty}^{\infty} H_n(x)\, H_m(x)\, \mathrm{e}^{-x^2}\, \mathrm{d}x \ .$$

In other words, the polynomials H_0, H_1, H_2, $\dots$, H_n constitute an orthogonal basis of the space $V_n(-\infty, \infty; \mathrm{e}^{-x^2})$. Here are the first five Hermite polynomials:

$$H_0(x) = 1 \ , \ \ H_1(x) = 2x \ , \ \ H_2(x) = 4x^2 - 2 \ , \ \ H_3(x) = 8x^3 - 12x \ , \ \ H_4(x) = 16x^4 - 48x^2 + 12 \ .$$

3 Gaussian quadrature

Theorem 1. *Let w be a weight function on $[a, b]$, let n be a positive integer, and let G_0, G_1, $\dots$, G_n be an orthogonal family of polynomials with degree of G_k equal to k for each $k = 0, 1, \dots, n$. In other words, G_0, G_1, $\dots$, G_n form an orthogonal basis of the inner product linear space $V_n(a, b; w)$. Let x_1, x_2, $\dots$, x_n be the roots of G_n, and define*

$$L_i(x) := \prod_{j=1,\ j \neq i}^{n} \frac{x - x_j}{x_i - x_j} \qquad \text{for} \ \ i = 1, 2, \dots, n \ .$$

Then the corresponding Gaussian quadrature formula is given by

$$I(f) := \int_a^b f(x)\, w(x)\, \mathrm{d}x \ \approx \ I_n(f) := \sum_{i=1}^{n} w_i\, f(x_i) \ ,$$

where

$$w_i := \int_a^b L_i(x)\, w(x)\, \mathrm{d}x \ .$$

The formula $I_n(f)$ has degree of precision exactly $2n - 1$, which means that $I_n(x^k) = I(x^k)$ for $k = 0, 1, \dots, 2n - 1$, but there is a polynomial Q of degree $2n$ for which $I_n(Q) \neq I(Q)$.