# 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*

*(A$_1$) associativity:* $\mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w} \quad \forall\ \mathbf{u},\ \mathbf{v},\ \mathbf{w}$ *in* $V$*;*

*(A$_2$) existence of a zero vector:* $\exists\ \mathbf{0} \in V$ *such that* $\mathbf{u} + \mathbf{0} = \mathbf{u} \quad \forall \mathbf{u} \in V$*;*

*(A$_3$) existence of an opposite element:* $\forall \mathbf{u} \in V\ \exists(-\mathbf{u}) \in V$ *such that* $\mathbf{u} + (-\mathbf{u}) = \mathbf{0}$*;*

*(A$_4$) 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*

*(B$_1$)* $\alpha(\mathbf{u} + \mathbf{v}) = \alpha\mathbf{u} + \alpha\mathbf{v} \quad \forall\ \alpha \in \mathbb{R}, \forall \mathbf{u}, \mathbf{v} \in V$*;*

*(B$_2$)* $(\alpha + \beta)\mathbf{u} = \alpha\mathbf{u} + \beta\mathbf{u} \quad \forall\ \alpha, \beta \in \mathbb{R}, \forall \mathbf{u} \in V$*;*

*(B$_3$)* $(\alpha\beta)\mathbf{u} = \alpha(\beta\mathbf{u}) \quad \forall\ \alpha, \beta \in \mathbb{R}, \forall \mathbf{u} \in V$*;*

*(B$_4$)* $1\mathbf{u} = \mathbf{u} \quad \forall \mathbf{u} \in V$*.*

**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

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

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 $\alpha P$ 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 $\le 4$) 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 $H_0$, $H_1$, $H_2$, ... 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 $H_0$, $H_1$, $H_2$, ..., $H_n$ 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 $G_0$, $G_1$, ..., $G_n$ be an orthogonal family of polynomials with degree of $G_k$ equal to $k$ for each $k = 0, 1, \dots, n$. In other words, $G_0$, $G_1$, ..., $G_n$ form an orthogonal basis of the inner product linear space $V_n(a, b; w)$. Let $x_1$, $x_2$, ..., $x_n$ be the roots of $G_n$, and define*

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

*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 $I_n(Q) \neq I(Q)$.*

**Proof:** We will prove that the quadrature formula

$$I_n(f) = \sum_{i=1}^{n} w_i\, f(x_i)$$

(where the weights $w_i$ are given by the formula above) has degree of precision exactly $2n-1$ in three steps:

Step 1: *The degree of precision of the quadrature formula is* $\geq n-1$.
Let $V_{n-1}$ stand for the linear space of all polynomials of degree not exceeding $n-1$ defined for $x \in [a, b]$. We need to prove that our quadrature formula is exact for any $R \in V_{n-1}$.
The polynomials $L_i(x)$, $i = 1, 2, \ldots, n$ are Lagrange polynomials of degree $n-1$ such that $L_i(x_k) = \delta_{ik}$ for all $k = 1, 2, \ldots, n$. This implies that

$$\sum_{i=1}^{n} R(x_i)\, L_i(x)$$

is the Lagrange polynomial of degree $n-1$ that interpolates the polynomial $R$ at the $n$ points $x_1$, $x_2$, …, $x_n$. Recalling that $R$ is a polynomial of degree of degree $n-1$, we conclude that

$$R(x) = \sum_{i=1}^{n} R(x_i)\, L_i(x) \qquad \forall\ x \in [a, b]\ .$$

Then we have

$$\begin{aligned} I(R) &= \int_a^b R(x)\, w(x)\, \mathrm{d}x = \int_a^b \left[\sum_{i=1}^{n} R(x_i)\, L_i(x)\right] w(x)\, \mathrm{d}x \\ &= \sum_{i=1}^{n} R(x_i) \left[\int_a^b L_i(x)\, w(x)\, \mathrm{d}x\right] = \sum_{i=1}^{n} R(x_i)\, w_i = I_n(R)\ , \end{aligned}$$

therefore the quadrature formula is exact for any polynomial $R$ of degree up to and including $n-1$, or, in other words, the degree of precision of the quadrature formula is $\geq n-1$.

Step 2: *The degree of precision of the quadrature formula is* $\geq 2n-1$.
Let $P$ be a polynomial of degree $\leq 2n-1$, i.e., $P \in V_{2n-1}$. Divide $P$ by $G_n$ (which is a polynomial of degree $n$ to obtain

$$P(x) = Q(x)\, G_n(x) + R(x)\ ,$$

where $Q \in V_{n-1}$ and $R \in V_{n-1}$. Since the polynomials $G_0$, $G_1$, $G_2$, …, $G_{n-1}$ form a basis of the linear space $V_{n-1}$, we can write $Q$ in the form

$$Q(x) = \sum_{i=0}^{n-1} q_i\, G_i(x)\ .$$

Then

$$
\begin{aligned}
I(P) &= I(Q\,G_n + R) = \int_a^b \left[Q(x)\,G_n(x) + R(x)\right]\, w(x)\,\mathrm{d}x \\
&= \int_a^b \left[\sum_{i=0}^{n-1} q_i\,G_i(x)\,G_n(x)\right] w(x)\,\mathrm{d}x + \int_a^b R(x)\,w(x)\,\mathrm{d}x \\
&= 0 + \int_a^b R(x)\,w(x)\,\mathrm{d}x = I(R)\ ,
\end{aligned}
$$

because all polynomials $G_0$, $G_1$, ..., $G_{n-1}$ are orthogonal to $G_n$ (with respect to the scalar product defined with the weight function $w$):

$$
(G_i, G_n) = \int_a^b G_i(x)\,G_n(x)\,w(x)\,\mathrm{d}x = 0 \qquad \forall\ i = 0, 1, 2, \ldots, n-1\ .
$$

Now recall that $R$ is a polynomial of degree $\leq n-1$ to conclude that $I(R) = I_n(R)$ according to what we proved in Step 1.
Since $x_i$ are roots of the polynomial $G_n$, it follows that

$$
P(x_i) = Q(x_i)\,G_n(x_i) + R(x_i) = 0 + R(x_i) = R(x_i)\ ,
$$

which implies that $I_n(R) = I_n(P)$. Combining these results, we obtain

$$
I(P) = I_n(P) \qquad \forall\ P \in V_{2n-1}\ .
$$

Step 3: *The degree of precision of the quadrature formula is* $2n-1$.
We already know that the degree of precision is at least $2n-1$, so to prove that it is *exactly* $2n-1$, it is enough to find *one* polynomial of degree $2n$ for which the quadrature formula is *not* exact. Note that the polynomial $G_n^2(x)$ has degree exactly $2n$, and that

$$
I(G_n^2) = \int_a^b G_n^2(x)\,w(x)\,\mathrm{d}x > 0 \tag{2}
$$

because the integrand, $G_n^2(x)\,w(x)$, is nonnegative and can be zero only at isolated points (a polynomial like $G_n^2$ has at most $2n$ roots, and $w$ can vanish only at isolated points by the definition of weight function).
But, since $x_i$ are roots of $G_n$ for $i = 1, 2, \ldots, n$, the quadrature formula gives

$$
I_n(G_n^2) = \sum_{i=1}^{n} w_i\,G_n^2(x_i) = 0\ . \tag{3}
$$

Comparing (2) and (3), we see that the quadrature formula is *not* exact for $G_n^2$. ■

In the proof of the above theorem, we implicitly used that $G_n$ has exactly $n$ *simple* roots, all of which are inside the interval $(a, b)$. This property is established rigorously in the following lemma.

**Lemma 1.** *Let $w$ be a weight function on $[a, b]$, let $n$ be a positive integer, and let $G_0$, $G_1$, …, $G_n$ be a family of polynomials such that the degree of $G_k$ is equal to $k$ for each $k = 0, 1, \ldots, n$, and $(G_i, G_j) = 0$ if $i \neq j$, where the scalar product is defined by (1).*

*Then for each $k = 0, 1, 2, \ldots, n$, the polynomial $G_k$ has exactly $k$ real roots which are simple and lie in the interval $(a, b)$.*

**Proof:** First we will prove the existence of real roots for $G_k$, and then we will count those roots.

Step 1: *Existence of real roots of $G_k$.*

Since the degree of $G_0$ is zero, it follows that $G_0(x) = \alpha \; \forall \, x \in [a, b]$ for some constant $\alpha \neq 0$. (If you don't understand why $\alpha \neq 0$, look at page 87 of the book.) Then, for $k \geq 1$,

$$0 = \int_a^b G_0(x)\, G_k(x)\, w(x)\, \mathrm{d}x = \alpha \int_a^b G_k(x)\, w(x)\, \mathrm{d}x \ ,$$

where the first equality holds due to orthogonality. However, since $w$ is positive on $[a, b]$ except possibly being equal to 0 at isolated points, and the integral $\int_a^b G_k(x)\, w(x)\, \mathrm{d}x$ is equal to zero, we conclude that the function $G_k$ must change sign in $(a, b)$. Since $G_k$ is a continuous function (all polynomials are continuous functions), the Intermediate Value Theorem guarantees that $G_k$ has a real root somewhere in $(a, b)$.

Step 2: *Counting the roots of $G_k$.*

Suppose that $G_k$ changes sign at exactly $j$ points $r_1$, $r_2$, …, $r_j$ in $(a, b)$ such that

$$a < r_1 < r_2 < \cdots < r_j < b \ .$$

Without loss of generality, assume that $G_k(x) > 0$ for $x \in (a, r_1)$. Then $G_k$ alternates sign on $(r_1, r_2)$, $(r_2, r_3)$, …, $(r_j, b)$. Define the auxiliary function

$$Z(x) \ := \ (-1)^j \prod_{i=1}^{j} (x - r_j) \ \in \ V_j \ .$$

By construction, $Z(x)$ and $G_k(x)$ have the same sign for all $x \in [a, b]$. From this it follows that

$$\int_a^b Z(x)\, G_k(x)\, w(x)\, \mathrm{d}x > 0 \ . \qquad (4)$$

Suppose that $j < k$. Since the polynomials $G_0$, $G_1$, $G_1$, ..., $G_j$ form a basis for $V_j$, there exist constants $z_0$, $z_1$, $z_2$, ..., $z_j$ such that

$$Z(x) = \sum_{i=0}^{j} z_i \, G_j(x) \ .$$

Substituting this expression into (4), we obtain

$$\begin{aligned} \int_a^b Z(x)\, G_k(x)\, w(x)\, \mathrm{d}x &= \int_a^b \left[ \sum_{i=0}^{j} z_i \, G_j(x) \right] G_k(x)\, w(x)\, \mathrm{d}x \\ &= \sum_{i=0}^{j} z_i \int_a^b G_j(x)\, G_k(x)\, w(x)\, \mathrm{d}x = 0 \ , \end{aligned}$$

where we have used that $j < k$, which implies that the polynomials $G_j$ and $G_k$ are orthogonal. The last equality clearly contradicts (4)! Hence the assumption that $j < k$ was wrong, i.e., we must have that $j \geq k$. However, since the degree of the polynomial $G_k$ is $k$, $G_k$ cannot have more than $k$ roots, which implies that $j = k$. ■

**Example:** As an example of application of the above Theorem, let us rederive the quadrature formula we derived in class, namely,

$$\int_{-1}^{1} f(x)\, \mathrm{d}x \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \ .$$

This formula can be obtained by using the Legendre polynomials $P_k$ defined on page 3. Take the polynomials $P_0(x) = 1$, $P_1(x) = x$, and $P_2(x) = x^2 - \frac{1}{3}$, which are an orthogonal basis in the linear space $V_2(-1, 1; w(x) \equiv 1)$. Since $n = 2$, we expect that the formula that we will obtain will have degree of precision $2n - 1 = 2(2) - 1 = 3$. As in the Theorem above, define $x_1 = -\frac{1}{\sqrt{3}}$ and $x_2 = \frac{1}{\sqrt{3}}$ to be the zeros of the polynomial $P_2$, define the polynomials (of degree $n - 1 = 2 - 1 = 1$)

$$L_1(x) = \frac{x - x_2}{x_1 - x_2} \ , \qquad L_2(x) = \frac{x - x_1}{x_2 - x_1} \ ,$$

and the weights

$$w_1 = \int_{-1}^{1} L_1(x)\, w(x)\, \mathrm{d}x = \int_{-1}^{1} \frac{x - x_2}{x_1 - x_2}\, 1\, \mathrm{d}x = \frac{1}{x_1 - x_2} \left( \frac{x^2}{2} - x_2 x \right) \Bigg|_{x=-1}^{1} = 1 \ ,$$

and, similarly, $w_2 = \int_{-1}^{1} L_2(x)\, w(x)\, \mathrm{d}x = \cdots = 1$, to obtain

$$I_2(f) = \sum_{i=1}^{2} w_i \, f(x_i) = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \ .$$

As an exercise, check that the degree of accuracy of this quadrature formula is indeed 3.