2.4.1 Legendre polynomials L_n as orthogonal polynomials

We consider the interval $[-1,1]$. On the space $C([-1,1])$ we define a scalar product by

$$(u,v) := \int_{-1}^{1} u(x)v(x)\,dx. \tag{2.3}$$

We seek a sequence of polynomials $L_n \in \mathcal{P}_n$, $n = 0, 1, \dots,$, with the following properties:

(i) $\{L_0, \dots, L_n\}$ is a basis of $\mathcal{P}_n$ (for each n)

(ii) L_n is orthogonal to the space $\mathcal{P}_{n-1}$, i.e,.

$$\langle L_n, v\rangle = 0 \qquad \forall v \in \mathcal{P}_{n-1}. \tag{2.4}$$

Such polynomials can be constructed inductively with a variant of the "Gram-Schmidt-orthogonalization": We choose [2],

$$\widetilde{L}_0(x) := 1, \qquad \widetilde{L}_1(x) := x.$$

We note that

$$\langle \widetilde{L}_1, \widetilde{L}_0\rangle = 0, \tag{2.5}$$

so that (2.4) is satisfied for $n = 1$.
For $\widetilde{L}_2 \in \mathcal{P}_2$ we make the ansatz

$$\widetilde{L}_2(x) = x\widetilde{L}_1(x) + r_1$$

for a polynomial $r_1 \in \mathcal{P}_1$ to be determined. Writing $r_1 = a_0\widetilde{L}_0 + a_1\widetilde{L}_1$ the orthogonality conditions (2.4) imply the two equations

$$0 \stackrel{!}{=} \langle \widetilde{L}_2, \widetilde{L}_0\rangle = \langle x\widetilde{L}_1(x), \widetilde{L}_0(x)\rangle + a_0 \underbrace{\langle \widetilde{L}_0, \widetilde{L}_0\rangle}_{>0} + a_1 \underbrace{\langle \widetilde{L}_1, \widetilde{L}_0\rangle}_{=0 \text{ b/c of } (2.5)},$$

$$0 \stackrel{!}{=} \langle \widetilde{L}_2, \widetilde{L}_1\rangle = \langle x\widetilde{L}_1(x), \widetilde{L}_1\rangle + a_0 \underbrace{\langle \widetilde{L}_0, \widetilde{L}_1\rangle}_{=0 \text{ b/c of } (2.5)} + a_1 \underbrace{\langle \widetilde{L}_1, \widetilde{L}_1\rangle}_{>0}.$$

for the coefficients a_0, a_1. This system of equations can obviously be solved and therefore $\widetilde{L}_2$ is determined. By construction, we have (2.4) for $n \le 2$.
Inductively, we make for $\widetilde{L}_3$ the ansatz $\widetilde{L}_3(x) = x\widetilde{L}_2(x) + r_2(x)$ for an $r_2 \in \mathcal{P}_2$. Again, (2.4) yields after writing $r_2(x) = \sum_{i=0}^{2} a_i\widetilde{L}_i(x)$ a linear system of equations for the a_i:

$$0 \stackrel{!}{=} \langle \widetilde{L}_3, \widetilde{L}_0\rangle = \langle x\widetilde{L}_1(x), \widetilde{L}_0\rangle + \sum_{j=0}^{2} a_j \langle \widetilde{L}_j, \widetilde{L}_0\rangle,$$

$$0 \stackrel{!}{=} \langle \widetilde{L}_3, \widetilde{L}_1\rangle = \langle x\widetilde{L}_1(x), \widetilde{L}_1\rangle + \sum_{j=0}^{2} a_j \langle \widetilde{L}_j, \widetilde{L}_1\rangle,$$

$$0 \stackrel{!}{=} \langle \widetilde{L}_3, \widetilde{L}_2\rangle = \langle x\widetilde{L}_1(x), \widetilde{L}_2\rangle + \sum_{j=0}^{2} a_j \langle \widetilde{L}_j, \widetilde{L}_2\rangle.$$

[2] since the "classical" Legendre polynomials L_n are scaled slightly differently (see below), we employ the notation $\widetilde{L}_n$

Again, since we already know (2.4) for $n \leq 2$, the system of equations simplifies to

$$0 \stackrel{!}{=} (\widetilde{L}_3, \widetilde{L}_i) = \langle x\widetilde{L}_2, \widetilde{L}_i \rangle + a_i \underbrace{\langle \widetilde{L}_i, \widetilde{L}_i \rangle}_{>0}, \qquad i = 0, 1, 2.$$

This yields the coefficients a_i and therefore $\widetilde{L}_3$. In this way, we can construct inductively the polynomials $\widetilde{L}_n \in \mathcal{P}_n$, $n = 0, 1, \ldots$. Our procedure yields the representation

$$\widetilde{L}_{n+1}(x) = x\widetilde{L}_n(x) - \sum_{i=0}^{n} \frac{1}{\langle \widetilde{L}_i, \widetilde{L}_i \rangle} \langle x\widetilde{L}_n, \widetilde{L}_i \rangle \widetilde{L}_i(x)$$

This can be simplified furthermore with the aid of (2.4):

$$\langle x\widetilde{L}_n(x), \widetilde{L}_i(x) \rangle = \langle \widetilde{L}_n(x), x\widetilde{L}_i(x) \rangle \stackrel{(2.4)}{=} 0 \quad \text{für } i + 1 \leq n - 1, \tag{2.6}$$

Hence, we arrive at the so-called "3-term recurrence relation"

$$\begin{aligned} \widetilde{L}_{n+1}(x) &= x\widetilde{L}_n(x) - \sum_{i=0}^{n} \frac{1}{\langle \widetilde{L}_i, \widetilde{L}_i \rangle} \langle x\widetilde{L}_n(x), \widetilde{L}_i(x) \rangle \widetilde{L}_i(x) & (2.7)\\ &\stackrel{(2.6)}{=} x\widetilde{L}_n(x) - \sum_{i=n-1}^{n} \frac{1}{\langle \widetilde{L}_i, \widetilde{L}_i \rangle} \langle x\widetilde{L}_n(x), \widetilde{L}_i(x) \rangle \widetilde{L}_i(x) & (2.8)\\ &= x\widetilde{L}_n(x) - \widetilde{a}_n \widetilde{L}_n(x) - \widetilde{b}_n \widetilde{L}_{n-1}(x) = (x - \widetilde{a}_n)\widetilde{L}_n(x) - \widetilde{b}_n \widetilde{L}_{n-1}(x), & (2.9) \end{aligned}$$

with

$$\widetilde{a}_n = \frac{\langle x\widetilde{L}_n(x), \widetilde{L}_n(x) \rangle}{\langle \widetilde{L}_n, \widetilde{L}_n \rangle}, \qquad \widetilde{b}_n = \frac{\langle x\widetilde{L}_n(x), \widetilde{L}_{n-1}(x) \rangle}{\langle \widetilde{L}_{n-1}, \widetilde{L}_{n-1} \rangle}.$$

Polynomials that satisfy the condition Polynome, die die Bedingungen (i), (ii) are not unique. For example, each L_n could be multiplied by a factor $c_n \neq 0$. However, this is the only freedom, i.e., each system L_n that satisfies the conditions (i), (ii) is of the form $L_n = c_n \widetilde{L}_n$ with the above constructed $\widetilde{L}_n$. The "classiscal" Legendre polynomials L_n are fixed by the "normalization condition" $l_n(1) = 1$. We have:

Theorem 2.13 (Legendre polynomials) *There holds:*

A. *There is a unique sequence $(L_n)_{n \in \mathbb{N}_0}$ of polynomials $L_n \in \mathcal{P}_n$, the* Legendre polynomials, *that satisfy the following conditions:*

   (i) $\{L_0, \ldots, L_n\}$ is a basis of $\mathcal{P}_n$ (for each n)

   (ii) L_n is orthogonal to the space $\mathcal{P}_{n-1}$, i.e., satisfies (2.4) for all $n \in \mathbb{N}_0$.

   (iii) $L_n(1) = 1$ for all $n \in \mathbb{N}_0$.

B. *The Legendre polynomials L_n have the explicit representation ("*Rodrigues formula*")*

$$L_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n \tag{2.10}$$

C. The Legendre polynomials satisfy the "3-term recurrence relation"

$$(n+1)L_{n+1}(x) = (2n+1)xL_n(x) - nL_{n-1}(x) \tag{2.11}$$

Proof: Item A has essentially been shown already. Items B, C are essential seen by direct computation—see the literature for details. □

Remark 2.14 *The 3-term recurrence (2.11) is the standard way to evaluate Legendre polynomials. The Legendre polynomials are a very important representative of the class of* orthogonal polynomials. *Other important families of orthogonal polynomials are the Chebyshev polynomials and the Jacobi polynomials. All orthogonal polynomials satisfy 3-term recurrence relations and are typically evaluated in this way.* ■

2.4.2 Gaussian quadrature

We will use the following result without proof:

Theorem 2.15 *For each $n \in \mathbb{N}_0$, the Legendre polynomial L_{n+1} has exactly $n+1$ (pairwise distinct) zeros $x_0, \ldots, x_n$. Furthermore, $x_i \in (-1,1)$ for all i.*

Proof: Literature. □

With the aid of the $n+1$ zeros of L_{n+1} we define the Gaussian quadrature as the "interpolatory" quadratur, i.e., we interpolate the integrand in the $n+1$ zeros of L_{n+1} and integrate the interpolating polynomial:

$$\text{Gauss points: } x^G_{i,n} = \text{zeros of } L_{n+1} \tag{2.12a}$$

$$\text{Gauss weights: } w^G_{i,n} = \int_{-1}^{1} \ell_i(x)\,dx, \qquad \ell_i(x) = \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x - x^G_{j,n}}{x^G_{i,n} - x^G_{j,n}} \tag{2.12b}$$

By construction, this is a quadrature formula $Q^{Gauss}_n(f) := \sum_{i=0}^n w^G_{i,n} f(x^G_{i,n})$ that is exact for polynomials of degree n:

$$\int_{-1}^{1} g(x)\,dx = Q^{Gauss}_n(g) \qquad \forall g \in \mathcal{P}_n \tag{2.13}$$

In fact, this rule is exact for polynomials of degree $2n+1$:

Theorem 2.16 (Gaussian quadrature) *The quadrature rule Q^{Gauss}_n defined (2.12) satisfies:*

$$Q^{Gauss}_n(f) = \int_{-1}^{1} f(x)\,dx \qquad \forall f \in \mathcal{P}_{2n+1} \tag{2.14}$$

$$w^G_{i,n} > 0 \qquad i = 0, \ldots, n. \tag{2.15}$$

Furthermore, there is no *quadrature rule with $n+1$ points that is exact for all polynomials of degree $2n+2$.*

Proof: *Proof of* (2.14)*:* Let $f \in \mathcal{P}_{2n+1}$. With the aid of polynomial division ("Euklidian algorithm")

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we write f as

$$f(x) = L_{n+1}(x)q_n(x) + r_n(x)$$

with two polynomials q_n, $r_n \in \mathcal{P}_n$. Then

$$\begin{aligned}\int_{-1}^{1} f(x)\,dx &= \underbrace{\int_{-1}^{1} L_{n+1}(x)q_n(x)\,dx}_{=0 \text{ wg. (2.4)}} + \int_{-1}^{1} r_n(x)\,dx \\ &= \int_{-1}^{1} r_n(x)\,dx \overset{(2.13)}{=} Q_n^{Gauss}(r_n) = \sum_{i=0}^{n} w_{i,n}^G r_n(x_{i,n}^G) \\ &\overset{L_{n+1}(x_{i,n}^G)=0}{=} \sum_{i=0}^{n} w_{i,n}^G L_{n+1}(x_{i,n}^G)q_n(x_{i,n}^G) + r_n(x_{i,n}^G) = Q_n^{Gauss}(f)\end{aligned}$$

Proof of (2.15)*:* We apply the quadrature formula to ℓ_i:

$$\begin{aligned}w_{i,n}^G &\overset{\ell_i(x_{j,n}^G)=\delta_{i,j}}{=} \sum_{j=0}^{n} w_{j,n}\ell_i(x_{j,n}^G) \overset{\ell_i(x_{j,n}^G)=\delta_{i,j}}{=} \sum_{j=0}^{n} w_{j,n}(\ell_i(x_{j,n}^G))^2 \\ &= Q_n^{Gauss}(\ell_i^2) \overset{\ell_i^2\in\mathcal{P}_{2n},(2.14)}{=} \int_{-1}^{1} \ell_i^2(x)\,dx > 0.\end{aligned}$$

Proof that no rule with $n+1$ points is exact for all polynomials of $\mathcal{P}_{2n+2}$: Let x_i, $i = 0, \ldots, n$, be the quadrature points of a rule. Consider

$$f(x) = \prod_{j=0}^{n}(x - x_i)^2 \in \mathcal{P}_{2n+2}$$

Then $0 < \int_{-1}^{1} f(x)\,dx$, but $Q_n(f) = 0$. □

Gaussian quadrature converges for integrands $f \in C([-1,1])$ if $n \to \infty$:

Theorem 2.17 (convergence of Gaussian quadrature) *There holds:*

$$\left|\int_{-1}^{1} f(x)\,dx - Q_n^{Gauss}(f)\right| \le 4 \min_{v\in\mathcal{P}_{2n+1}} \|f - v\|_{\infty,[-1,1]}. \tag{2.16}$$

In particular there holds $\int_{-1}^{1} f(x)\,dx = \lim_{n\to\infty} Q_n^{Gauss}(f)$ for each $f \in C([-1,1])$.

Proof: As in the proof of Theorem 2.7 we exploit that the quadrature rule is exact for polynomials of a particular degree. For arbitrary $v \in \mathcal{P}_{2n+1}$ we have

$$\begin{aligned}\int_{-1}^{1} f(x)\,dx - Q_n^{Gauss}(f) &\overset{\text{Satz 2.16}}{=} \int_{-1}^{1} (f(x) - v(x))\,dx + Q_n^{Gauss}(v) - Q_n^{Gauss}(f) \\ &= \int_{-1}^{1} (f(x) - v(x))\,dx + Q_n^{Gauss}(v - f)\end{aligned}$$

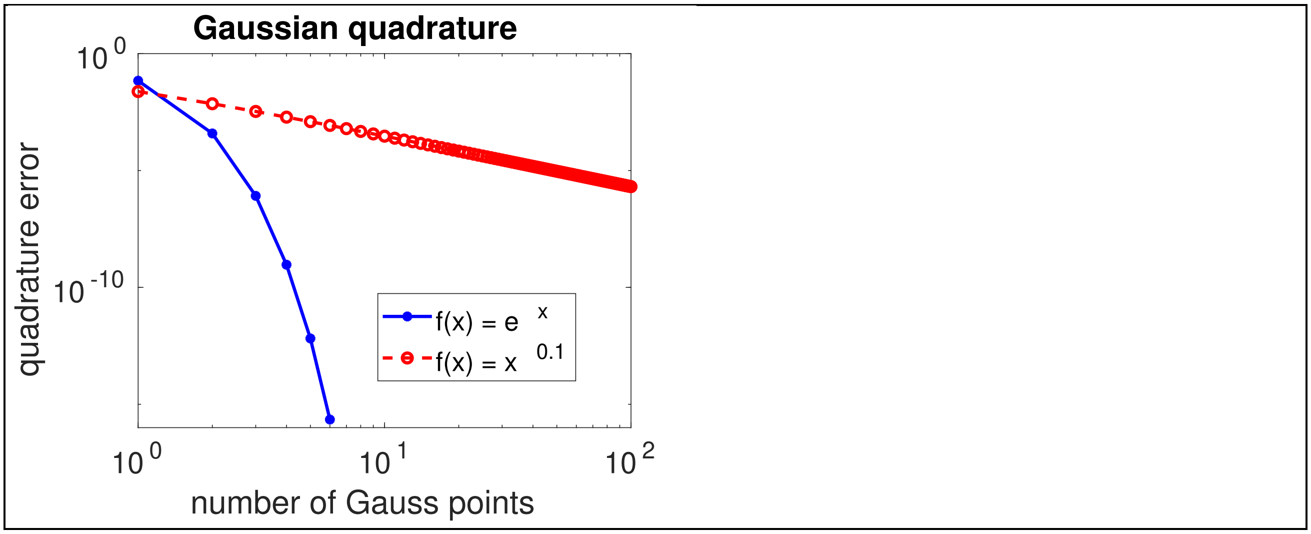

Figure 2.4: Gaussian quadrature on the interval $[0, 1]$ for smooth integrand $f(x) = \exp(x)$ and non-smooth integrand $f(x) = x^{0.1}$.

and therefore (note: $\sum_{i=0} w^G_{i,n} = Q^{Gauss}_n(1) = \int_{-1}^1 1\,dx = 2$)

$$
\begin{aligned}
\left|\int_{-1}^1 f(x)\,dx - Q^{Gauss}_n(f)\right| &\leq \left|\int_{-1}^1 f(x) - v(x)\,dx\right| + \left|Q^{Gauss}_n(f-v)\right| \\
&\leq 2\|f-v\|_{\infty,[-1,1]} + \sum_{i=0}^n \underbrace{|w^G_{i,n}|}_{=w^G_{i,n} \text{ b/c of } (2.15)} \underbrace{|f(x^G_{i,n}) - v(x^G_{i,n})|}_{\leq \|f-v\|_{\infty,[-1,1]}} \\
&\leq (2 + \sum_{i=0}^n w^G_{i,n})\|f-v\|_{\infty,[-1,1]} = 4\|f-v\|_{\infty,[-1,1]}.
\end{aligned}
$$

Since $v \in \mathcal{P}_{2n+1}$ was arbitrary, we may pass to the minimum and arrive at the claim. □

Gaussian quadrature is very efficient for *smooth* integrands:

Example 2.18 *We consider Gaussian quadrature with $n+1$ points on the interval $[0, 1]$ (i.e., the quadrature points are $x_i = \frac{1}{2}(1 + x^G_{i,n})$ and the weights $w_i = \frac{1}{2}w^G_{i,n}$) for $f_1(x) = \exp(x)$ and $f_2(x) = x^{0.1}$. While very rapid convergence is visible for the smooth integrand f_1, Gaussian quadrature is not very efficient for the non-smooth integrand f_2.*
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■

Typically, Gaussian quadrature is also employed in composite rules. Then the number $n+1$ of Gaussian points (per subinterval) is typically fixed. Convergence results analogous to those for the composite trapezoidal and Simpson rule of Theorem 2.7 hold true.

Remark 2.19 *There is no explicit formula for the Gauss points and weigths for $n \geq 5$. There are may implementations, e.g.,* `gauleg.c` *from "Numerical Recipes" (also available as* `gauleg.m`*)) or* `numpy.polynomial.legendre.leggauss`. ■

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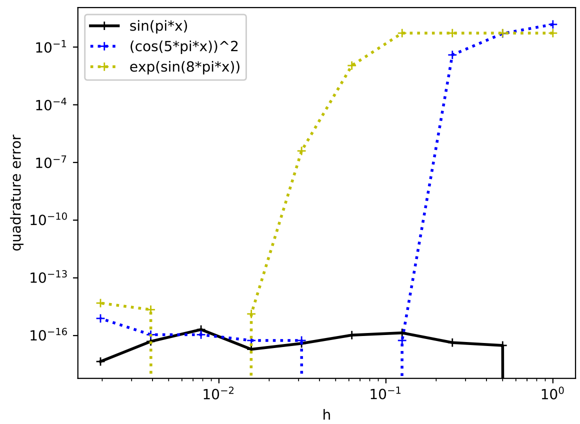

Figure 2.5: Composite trapezoidal rule on $[-1,1]$ for $f_1(x) = \sin(\pi x)$, $f_2(x) = (\cos(\pi x))^{10}$, $f_3(x) = \exp(\sin(8\pi x))$.

2.5 Comments on the trapezoidal rule

The (composite) Gauss rules are much more efficient than then composite trapezoidal rule for smooth integrands. There is one exception: the integration of smooth *periodic* functions over one period. In this case, the trapezoidal rule converges very rapidly and is typically employed:

Example 2.20 *We employ the composite trapezoidal rule for the numerical integration on* $[-1,1]$ *for the following three periodic functions:*

$$f_1(x) = \sin(\pi x), \qquad f_2(x) = (\cos(\pi x))^{10}, \qquad f_3(x) = \exp(\sin(8\pi x)).$$

We observe in Fig. 2.5: the composite trapezoidal rule is exact for rather large step sizes h for f_1; for somewhat large step sizes it is exact for the trigonometric polynomial f_2; for f_3 we also observe fast convergence.

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■

2.6 Quadrature in 2D

Goal: Determine $\int_T f(x)\,dx$, where $T \subset \mathbb{R}^2$ is the reference triangle $T = \{(x,y)\,|\,0 < x < 1, 0 < y < 1-x\}$ or the reference square $S = (0,1)^2$.
In principle, the typical construction of quarature rule for triangles or rectangles follows that in 1D: one selects quadrature points and weights in such a way that certain polynomials are integrated exactly.

2.6.1 Quadrature on squares

A quadrature rule for the square S is typically obtained from a 1D rule by a product construction. To that end, let

$$Q_n^{1D}(f) := \sum_{i=0}^{n} w_i f(x_i) \approx \int_0^1 f(x)\,dx \tag{2.17}$$

be a 1D rule. Then, one can define for functions $F(x,y)$ the 2D rule

$$Q_n^{2D}(F) := \sum_{i,j=0}^{n} w_i w_j F(x_i, x_j). \tag{2.18}$$

Exercise 2.21 *Let the 1D rule (2.17) be exact for polynomials of degree p, i.e., $Q_n^{1D}(f) = \int_0^1 f(x)\,dx$ for all $f \in \mathcal{P}_p$. Then the rule Q_n^{2D} is exact for all polynomials $F \in \operatorname{span}\{(x^i y^j \,|\, i,j = 0,\ldots,p\}$.* ■

2.6.2 Quadrature on triangles

Quadrature rules on the triangle T are typically created in one of the following two ways:

1. One selects points in T. The condition that certain polynomials are integrated exactly determines the quadrature weights.
2. The triangle T is transformed to a square and a quadrature formula for the square S is employed.

Exercise 2.22 *The simplest case is a quadrature rule with 1 point, e.g., the barycenter of T. What is the corresponding quadrature weight so that the rule exact for polynomials of degree 0? Show that this is rule is in fact exact for polynomials of degree 1, i.e., for polynomials $F(x,y) = a + bx + cy$.*
The next case is a quadrature rule with 3 points, e.g., the vertices of T. Construct the weights such that the rule is exact for polynomials of degree 1. ■

Example 2.23 *Let Q^{2D} be a quadrature rule on S with N points $\mathbf{x}_i = (x_i, y_i) \in S$ and corresponding weights w_i, $i = 0,\ldots,N$. The substitution ("Duffy transformation")*

$$\int_T F(x,y)\,dy\,dx = \int_{x=0}^1 \int_{y=0}^{1-x} F(x,y)\,dy\,dx = \int_{x=0}^1 \int_{\eta=0}^1 F(x,(1-x)\eta)(1-x)\,d\eta\,dx$$

suggests the following quadrature rule on T:

$$\int_T F(x,y)\,dy\,dx = \int_{x=0}^1 \int_{\eta=0}^1 F(x,(1-x)\eta)(1-x)\,d\eta\,dx \approx \sum_i F(x_i,(1-x_i)y_i)(1-x_i)w_i.$$

Typically, rules Q^{2D} for S are derived from 1D rules as described in Section 2.6.1. The 1D rule can be a Newton-Cotes formula or a Gauss rule or a composite Newton-Cotes or Gauss rule. ■

2.6.3 Further comments

Integrals over "arbitray" domains $G \subset \mathbb{R}^2$ are typically done by composite rules, in which G is decomposed into triangles or quadrilaterals and each subdomain is then treated by a rule of the above type.