CHAPTER 2

The Abstract Framework

Our study of quadrature theory begins with a very general framework, formulated mainly in terms of linear algebra, which will help us to discern the fundamental notions and principles. In this chapter we derive results that shed light on the place occupied by quadrature rules within the collection of all algorithms for computing a definite integral based on a common set of information. These results will serve to justify our focusing attention on quadrature rules in the rest of the book.

2.1. Standard estimation framework

DEFINITION 2.1.1. A *standard estimation framework* (SEF) comprises:

(1) a real linear space V;
(2) a linear functional I defined on V;
(3) a linear map $O : V \to \mathbb{R}^n$ (observation); and
(4) a non-empty convex symmetric[1] set $\mathcal{C} \subset V$ (co-observation).

In what follows, we shall always assume an SEF. In this context, we wish to approximate $I[f]$ based solely on knowledge of $O[f]$ and the assumption that $f \in \mathcal{C}$. As outlined in Chapter 1, in quadrature theory we use a special SEF with:

(1) $V = C[a, b]$;
(2) $I[f] = \int_a^b f(x)w(x)\,dx$, where w is a fixed integrable function;
(3) $O[f] = \big(f(x_1), \ldots, f(x_n)\big)$; and
(4) various choices of $\mathcal{C}$.

The main body of quadrature theory is based on such SEFs. Sometimes we generalize the observation by including values of derivatives as additional information, which is a reasonable thing to do if these values are obtainable at low computational cost, for example as known Taylor coefficients. Another type of observation that is occasionally of practical interest consists of mean values of f over small intervals; see Omladič *et al.* (1976), Pittnauer and Reimer (1979), Omladič (1992), Motornyi (1998) and Bojanov and Petrov (2001, 2005).

By varying V, I, O and $\mathcal{C}$, a broad spectrum of problems in numerical mathematics can be subsumed under the notion of an SEF, for example interpolation ($I[f] := f(u)$ with u fixed), numerical differentiation ($I[f] = f'(u)$ with u fixed), and the computation of Cauchy principal value integrals, line integrals, volume integrals etc.

[1]A symmetric set $\mathcal{C}$ is such that $-\mathcal{C} = \mathcal{C}$, i.e. $-f \in \mathcal{C} \iff f \in \mathcal{C}$.

Considering problems within an SEF enables us to compare algorithms and make precise the meaning of a "best" algorithm. The central idea is that there exists some information or the possibility of obtaining some kind of information, and we should make the best of it. The theory of information-based complexity (see, e.g., Woźniakowski 1985, Traub *et al.* 1988 or Novak 1988) discusses problems of this sort from a more general standpoint.

Next, let us define our available information.

DEFINITION 2.1.2. For $f \in \mathcal{C}$,

$$\mathrm{Info}(f) := \{g : O[g] = O[f]\} \cap \mathcal{C}.$$

The aim now is to calculate the set

$$I[\mathrm{Info}(f)]$$

of all possible values of I that are compatible with the given information $\mathrm{Info}(f)$. Since $\mathrm{Info}(f)$ is the intersection of two convex sets and hence also convex, and since I is linear, the set $I[\mathrm{Info}(f)]$ is an interval. We characterize this interval by its endpoints.

DEFINITION 2.1.3. For $z \in O(\mathcal{C})$,

$$\begin{aligned} \hat{Q}[z] &:= \sup\{I[f] : O[f] = z,\ f \in \mathcal{C}\}, \\ \underset{\vee}{Q}[z] &:= \inf\{I[f] : O[f] = z,\ f \in \mathcal{C}\}. \end{aligned}$$

Often we shall write simply $\underset{\vee}{Q}[f]$ in place of $\underset{\vee}{Q}(O[f])$, but it is important to remember that $\underset{\vee}{Q}$ is defined on $O(\mathcal{C}) \subset \mathbb{R}^n$, and similarly for $\hat{Q}$.

We are interested in situations where the error of at least one algorithm can be bounded by a finite number. Therefore, the interval $I[\mathrm{Info}(f)]$ of all possible values has to be bounded.

General Assumption. *Unless explicitly stated otherwise, we shall always assume that we are in an SEF where for each* $f \in \mathcal{C}$, $\hat{Q}[f] < \infty$ *and* $\underset{\vee}{Q}[f] > -\infty$.

The best we can do in this situation is to choose the midpoint of $I[\mathrm{Info}(f)]$ as an estimate for $I[f]$. This estimate can deviate from the true value by at most half of the width of $I[\mathrm{Info}(f)]$, and no smaller deviation can be guaranteed for any estimate.

DEFINITION 2.1.4. The *strongly optimal estimate* is

$$Q^{\mathrm{so}}[f] := \frac{1}{2}\left(\hat{Q}[f] + \underset{\vee}{Q}[f]\right).$$

The *intrinsic error* is

$$\rho^{\mathrm{intr}}[f] := \frac{1}{2}\left(\hat{Q}[f] - \underset{\vee}{Q}[f]\right),$$

and the *error of the SEF* is defined by

$$\rho^{\mathrm{opt}} := \sup\{\rho^{\mathrm{intr}}[f] : f \in \mathcal{C}\}.$$

We can view ρ^{opt} as the *a priori* error of the estimation problem, i.e. the smallest uncertainty that can be guaranteed by an appropriate algorithm before the evaluation of $O[f]$. This quantity can be used for, among other things, evaluating the observation functional O. On the other hand, $\rho^{\text{intr}}[f]$ is the *a posteriori* error bound.

Before we try to understand the notions introduced so far via an example, let us point out the equality

$$Q_{\vee}[f] = -\hat{Q}[-f], \tag{2.1}$$

which follows readily from the linearity of I and the symmetry of $\mathcal{C}$.

Example 2.1.1 (Secrest 1964). We study the SEF given by

(1) $V = C[a,b]$;
(2) $I[f] = \int_a^b f(x)\,dx$;
(3) $O[f] = \big(f(x_1), \dots, f(x_n)\big)$ where $a \le x_1 < x_2 < \dots < x_n \le b$;
(4) $\mathcal{C} = \text{Lip}_M 1 := \big\{f : |f(x) - f(y)| \le M|x-y| \text{ for } x, y \in [a,b]\big\}$.

For $x \in [x_\nu, x_{\nu+1}]$, $f \in \mathcal{C}$ yields

$$f(x) - f(x_\nu) \le M(x - x_\nu), \tag{2.2}$$
$$f(x) - f(x_{\nu+1}) \le M(x_{\nu+1} - x), \tag{2.3}$$

which means that

$$f(x) \le \min\big\{f(x_\nu) + M(x - x_\nu),\ f(x_{\nu+1}) + M(x_{\nu+1} - x)\big\}.$$

Let x^* be such that $f(x_\nu) + M(x^* - x_\nu) = f(x_{\nu+1}) + M(x_{\nu+1} - x^*)$. On the interval $[x_\nu, x^*]$ the first bound (2.2) is smaller, while on $[x^*, x_{\nu+1}]$ the second bound (2.3) is smaller. We choose the better bound in each case and obtain

$$\int_{x_\nu}^{\mathrm{x}_{\nu+1}} f(x)\,dx \le \frac{x_{\nu+1} - x_\nu}{2}[f(x_{\nu+1}) + f(x_\nu)] + \frac{M}{4}(x_{\nu+1} - x_\nu)^2 - \frac{[f(x_{\nu+1}) - f(x_\nu)]^2}{4M}. \tag{2.4}$$

Using analogous estimates on the intervals $[a, x_1]$ and $[x_n, b]$, we get

$$\begin{aligned} \hat{Q}[f] \le\ & f(x_1)(x_1 - a) + \frac{M}{2}(x_1 - a)^2 + \sum_{\nu=1}^{n-1} \frac{(x_{\nu+1} - x_\nu)}{2}[f(x_{\nu+1}) + f(x_\nu)] \\ & + \frac{M}{4}\sum_{\nu=1}^{n-1}(x_{\nu+1} - x_\nu)^2 - \frac{1}{4M}\sum_{\nu=1}^{n-1}[f(x_{\nu+1}) - f(x_\nu)]^2 \\ & + f(x_n)(b - x_n) + \frac{M}{2}(b - x_n)^2. \end{aligned}$$

In fact, equality holds. This can be seen by constructing a broken line function $f_o \in \text{Info}(f)$ such that equality holds in (2.2) and (2.3) on the respective intervals.

A similar expression for $\check{Q}[f]$ follows from (2.1). Finally, we obtain

$$\begin{aligned} Q^{\mathrm{so}}[f] &\\ &= f(x_1)(x_1-a) + \sum_{\nu=1}^{n-1} \frac{x_{\nu+1}-x_\nu}{2}[f(x_{\nu+1}+f(x_\nu)] + f(x_n)(b-x_n) \\ &= \left(\frac{x_1+x_2}{2}-a\right) f(x_1) + \sum_{\nu=2}^{n-1} \frac{x_{\nu+1}-x_{\nu-1}}{2} f(x_\nu) + \left(b - \frac{x_{n-1}+x_n}{2}\right) f(x_n). \end{aligned}$$

We call this algorithm the "generalized trapezoidal rule"; it will come up frequently. For the special case where $x_\nu = a + (\nu - \frac{1}{2})(b-a)/n$, we obtain the "midpoint rule"

$$Q_n^{\mathrm{Mi}}[f] := \frac{b-a}{n} \sum_{\nu=1}^{n} f(x_\nu), \tag{2.5}$$

whereas $x_\nu = a + (\nu-1)(b-a)/(n-1)$ gives the usual "trapezoidal rule"

$$Q_n^{\mathrm{Tr}}[f] := \frac{b-a}{n-1} \left[\frac{1}{2} f(a) + \sum_{\nu=2}^{n-1} f(x_\nu) + \frac{1}{2} f(b)\right].$$

In the general case, note that

$$\begin{aligned} \rho^{\mathrm{intr}}[f] = \frac{M}{2}(x_1-a)^2 + \frac{M}{4} \sum_{\nu=1}^{n-1} (x_{\nu+1}-x_\nu)^2 \\ - \frac{1}{4M} \sum_{\nu=1}^{n-1} [f(x_{\nu+1}) - f(x_\nu)]^2 + \frac{M}{2}(b-x_n)^2 \end{aligned}$$

and therefore

$$\rho^{\mathrm{opt}} = \frac{M}{4}\left[2(x_1-a)^2 + \sum_{\nu=1}^{n-1}(x_{\nu+1}-x_\nu)^2 + 2(b-x_n)^2\right].$$

Here is a useful property of the quantities introduced above.

LEMMA 2.1.1. $\check{Q}$ is a convex function while $\hat{Q}$ and ρ^{intr} are concave functions on $\mathcal{C}$.

PROOF. For given $f_1, f_2 \in \mathcal{C}$ and $\varepsilon > 0$, there exist $g_i \in \mathrm{Info}(f_i)$ satisfying

$$\check{Q}[f_i] + \varepsilon \geq I[g_i] \quad \text{for } i = 1, 2,$$

and for arbitrary $\alpha \in [0,1]$ we have

$$\begin{aligned} \check{Q}[\alpha f_1 + (1-\alpha) f_2] &\leq I[\alpha g_1 + (1-\alpha) g_2] = \alpha I[g_1] + (1-\alpha) I[g_2] \\ &\leq \alpha\, \check{Q}[f_1] + (1-\alpha)\, \check{Q}[f_2] + \varepsilon. \end{aligned} \tag{2.6}$$

Convexity of $\check{Q}$ follows, since the inequalities in (2.6) hold for each $\varepsilon > 0$. The concavity of $\hat{Q}$ follows in a similar fashion, and ρ^{intr} is concave because it is the difference of a concave function and a convex one. □

An important consequence is the following theorem, which says that the zero vector is the worst possible observation.

THEOREM 2.1.1. Denote by 0 the zero element of V. Then

$$\rho^{\text{opt}} = \rho^{\text{intr}}[0] = \sup\{I[f] \,:\, f \in \mathcal{C} \cap \operatorname{Ker} O\}. \tag{2.7}$$

PROOF. Let us first note that there exists an $f \in \mathcal{C}$ and that, by convexity and symmetry, we also have $0 = [f + (-f)]/2 \in \mathcal{C}$. From equation (2.1), we obtain that for each $f \in \mathcal{C}$,

$$\rho^{\text{intr}}[f] = \rho^{\text{intr}}[-f].$$

Thus, the concavity of ρ^{intr} gives

$$\rho^{\text{intr}}[0] = \rho^{\text{intr}}[(f + (-f))/2] \geq \frac{1}{2}\Big(\rho^{\text{intr}}[f] + \rho^{\text{intr}}[-f]\Big) = \rho^{\text{intr}}[f],$$

which proves the first equality in (2.7). The second equality follows immediately from (2.1). □

The next result shows that, in order to determine $I[\text{Info}(f)]$ for a given $f \in \mathcal{C}$, it is sufficient to investigate linear algorithms. By a linear algorithm we mean an algorithm that maps $O[f]$ linearly into $\mathbb{R}$. Since $O[f] \in \mathbb{R}^n$, such an algorithm can be represented by an element of $A \in \mathbb{R}^n$. For convenience, we use the notation

$$AO[f] := A \cdot (O[f])^{\mathrm{T}}.$$

In the following, we shall use some results from the geometry of convex sets; see, for instance, Webster (1994). We denote by $\operatorname{ri}(K)$ the relative interior of the convex set K, i.e. the set of interior points if we view K as a subset of its affine hull.

THEOREM 2.1.2 (Heindl 1982). Let $f \in \mathcal{C}$ and $O[f] \in \operatorname{ri}(O[\mathcal{C}])$. Then

$$\hat{Q}[f] = \inf_{A \in \mathbb{R}^n} \left\{ AO[f] + \sup_{g \in \mathcal{C}} \big(I[g] - AO[g]\big) \right\}, \tag{2.8}$$

$$\underset{\vee}{Q}[f] = \sup_{A \in \mathbb{R}^n} \left\{ AO[f] + \inf_{g \in \mathcal{C}} \big(I[g] - AO[g]\big) \right\}. \tag{2.9}$$

Moreover, the infimum and supremum over $A \in \mathbb{R}^n$ are attained.

PROOF. By a standard result on convex functions, there exists a hyperplane supporting $\underset{\vee}{Q}$ at $O[f]$, i.e. a linear mapping $A : \mathbb{R}^n \to \mathbb{R}$ that satisfies

$$\underset{\vee}{Q}[h] \geq AO[h - f] + \underset{\vee}{Q}[f] \tag{2.10}$$

for all $h \in \mathcal{C}$. Hence

$$\begin{aligned} \underset{\vee}{Q}[f] &\leq AO[f] + \underset{\vee}{Q}[h] - AO[h] \\ &= AO[f] + \inf\{I[g] - AO[g] \,:\, g \in \text{Info}(h)\}, \end{aligned}$$

and this holds for all $h \in \mathcal{C}$ such that

$$\underset{\vee}{Q}[f] \leq \sup_{A \in \mathbb{R}^n} \Big\{ AO[f] + \inf_{g \in \mathcal{C}} (I[g] - AO[g]) \Big\}.$$

On the other hand, for each $A \in \mathbb{R}^n$ we have

$$\begin{aligned} \check{Q}[f] &= AO[f] + \inf\{I[g] - AO[g] \, : \, g \in \mathrm{Info}(f)\} \\ &\geq AO[f] + \inf\{I[g] - AO[g] \, : \, g \in \mathcal{C}\} \end{aligned}$$

and, in particular,

$$\check{Q}[f] \geq \sup_{A \in \mathbb{R}^n} \big\{ AO[f] + \inf_{g \in \mathcal{C}} (I[g] - AO[g]) \big\}.$$

Equation (2.9) is therefore proved, with equality holding for the $A \in \mathbb{R}^n$ given in (2.10). The proof for $\hat{Q}[f]$ is similar. □

The applicability of this theorem is demonstrated by the following example.

Example 2.1.2 (von Mises 1933). Let
(1) $V = C[-1, 1]$;
(2) $I[f] = \int_{-1}^{1} f(x)\,dx$;
(3) $O[f] = \big(f(-1), f(0), f(1)\big)$; and
(4) $\mathcal{C} = \{f : \sup_{-1 \leq x \leq 1} |f''(x)| \leq M\}$.

The SEF so defined is rather special, but the method that follows can easily be generalized (though the calculations may become much more involved).

First let us note that the General Assumption is satisfied; that is, elements of $\mathrm{Info}(f)$ cannot have arbitrarily large integrals. Take $\xi \in [-1, 1]$; then for $f \in \mathcal{C}$ we have

$$\left| \frac{f(\xi) - f(-1)}{\xi + 1} - \frac{f(1) - f(\xi)}{1 - \xi} \right| \leq 2M.$$

Multiplying through by $|(1 - \xi)(1 + \xi)| \leq 1$ and using the triangle inequality yields

$$|f(\xi)| \leq M + \tfrac{1}{2}\big|f(-1)(1 - \xi) + f(1)(1 + \xi)\big| \leq M + \max\{|f(-1)|,\ |f(1)|\}.$$

Now let $O[f] \in \mathrm{ri}(O[\mathcal{C}])$. We have to determine

$$\hat{Q}[f] = \inf_{A \in \mathbb{R}^3} \Big\{ AO[f] + \sup_{g \in \mathcal{C}} \big(I[g] - AO[g]\big) \Big\},$$

and then we can apply equation (2.1).

For $p \in \mathbb{P}_1$ and arbitrary $\alpha \in \mathbb{R}$, we have that $\alpha p \in \mathbb{P}_1$ also. Hence, if $I[p] - AO[p] \neq 0$ for a polynomial $p \in \mathbb{P}_1$, we obtain

$$\sup_{f \in \mathcal{C}} \big(I[f] - AO[f]\big) = \infty.$$

Therefore such A are not of interest. An easy calculation shows that any other $A \in \mathbb{R}^3$ can be written as

$$AO[f] = 2f(0) + \eta D[f] \quad \text{where } D[f] := f(-1) - 2f(0) + f(1).$$

The functional AO is a method for estimating the functional I, so $I - AO$ represents its associated error. A systematic error theory, the so-called Peano kernel theory (see Section 4.2), shows that

$$\sup_{f \in \mathcal{C}} \big(I[f] - AO[f]\big) = \begin{cases} (1 - 3\eta)M/3 & \text{if } \eta \leq 0, \\ (8\eta^3 - 3\eta + 1)M/3 & \text{if } 0 \leq \eta \leq 1/2, \\ (3\eta - 1)M/3 & \text{if } \eta \geq 1/2. \end{cases}$$

Equation (2.8) then gives

$$\hat{Q}[f] = 2f(0) + \frac{M}{3} - \frac{2M}{3}\left(\frac{M - D[f]}{2M}\right)^{3/2}$$

and, finally,

$$\text{(2.11)} \qquad Q^{\text{so}}[f] = 2f(0) + \frac{M}{3}\left[\left(\frac{M + D[f]}{2M}\right)^{3/2} - \left(\frac{M - D[f]}{2M}\right)^{3/2}\right],$$

$$\text{(2.12)} \qquad \rho^{\text{intr}}[f] = \frac{M}{3} - \frac{M}{3}\left[\left(\frac{M + D[f]}{2M}\right)^{3/2} + \left(\frac{M - D[f]}{2M}\right)^{3/2}\right],$$

$$\text{(2.13)} \qquad \rho^{\text{opt}} = \frac{2 - \sqrt{2}}{6}\,M.$$

The condition $O[f] \in \text{ri}(O[\mathcal{C}])$ is equivalent to $|D[f]| < M$. It is obvious that the result can be extended to all $f \in \mathcal{C}$ satisfying $|D[f]| = M$. Therefore, we have full generality.

Up to now, we have endeavoured to make full use of our information Info(f). However, there are other criteria that can be used to evaluate algorithms. It will be necessary to consider algorithms other than Q^{so}, since our simple example already shows that calculation of Q^{so} may be difficult. In fact, there are very few situations in which Q^{so} is known explicitly.

Definition 2.1.5. Let A be a real function defined on $O(\mathcal{C})$. Then

$$Q := A \circ O$$

is called an *estimation rule*. The set of all estimation rules will be denoted by $\mathbf{Q}^{\text{gen}}$. The (worst-case) *error* of an estimation rule $Q \in \mathbf{Q}^{\text{gen}}$ is defined to be

$$\rho(Q) := \sup_{f \in \mathcal{C}} \big| I[f] - Q[f] \big|.$$

Note that errors of linear estimation rules have already, in some sense, played a role in Theorem 2.1.2. Another example is

$$\text{(2.14)} \qquad \rho(Q^{\text{so}}) = \rho^{\text{opt}}.$$

Estimation rules with the above property earn their own name:

Definition 2.1.6. An estimation rule $Q^{\text{opt}} \in \mathbf{Q}^{\text{gen}}$ is said to be *optimal* if

$$\rho(Q^{\text{opt}}) = \inf\{\rho(Q) : Q \in \mathbf{Q}^{\text{gen}}\}.$$

Theorem 2.1.3.

$$\text{(2.15)} \qquad \rho^{\text{opt}} = \inf\{\rho(Q) : Q \in \mathbf{Q}^{\text{gen}}\}.$$

Proof. Let $f \in \mathcal{C}$. From the definition of Q^{so} we obtain that for arbitrary $Q \in \mathbf{Q}^{\text{gen}}$,

$$\big[Q^{\text{so}}[f] - \rho^{\text{intr}}[f],\ Q^{\text{so}}[f] + \rho^{\text{intr}}[f]\big] \subseteq \big[Q[f] - \rho(Q),\ Q[f] + \rho[Q]\big].$$

Thus $\rho^{\text{intr}}[f] \leq \rho(Q)$ and hence $\rho^{\text{opt}} \leq \rho(Q)$. Since Q was arbitrary, the left-hand side of (2.15) does not exceed the right-hand side. Equality follows from (2.14). □

The estimation rule Q^{so}, while always optimal, is often complicated. A key result is that among all the optimal rules there is always a simple one.

DEFINITION 2.1.7. The estimation rule $Q = A \circ O$ is said to be *linear* if A is a linear map defined on $\mathbb{R}^n$. We denote the set of all linear estimation rules by $\mathbf{Q}$.

THEOREM 2.1.4 (Smolyak 1965). For each SEF, there exists a linear estimation rule that is optimal.

PROOF. Note that $(0, \dots, 0) \in \operatorname{ri}(O[\mathcal{C}])$. Taking $f \equiv 0$ in Theorem 2.1.2, we obtain the existence of an $A \in \mathbb{R}^n$ satisfying

$$\hat{Q}[0] = \sup_{g \in \mathcal{C}} \big(I[g] - AO[g]\big).$$

Theorem 2.1.1 then yields

$$\rho^{\text{opt}} = \rho^{\text{intr}}(0) = \tfrac{1}{2}\big[\hat{Q}[0] - \underset{\vee}{Q}(0)\big] = \hat{Q}(0).$$

The above two equations combined with the symmetry of $\mathcal{C}$ give the theorem. $\square$

We now know that for any estimation rule, we cannot guarantee a smaller *a priori* error than for the best linear rule—linear rules seem to be the simplest reasonable estimation rules. Therefore, in what follows, it makes sense to consider (almost) exclusively linear estimation rules.

The problems of uniqueness and construction of optimal linear rules are often difficult. Sometimes the following result may be helpful.

THEOREM 2.1.5. If

$$\lim_{\varepsilon \to 0} \frac{\rho^{\text{intr}}[\varepsilon f] - \rho^{\text{intr}}[0]}{\varepsilon} = 0$$

for all $f \in \mathcal{C}$, then there exists exactly one linear optimal rule Q^{opt}, and for all $f \in \mathcal{C}$ we have

$$\lim_{\varepsilon \to 0} \frac{Q^{\text{so}}[\varepsilon f]}{\varepsilon} = Q^{\text{opt}}[f].$$

PROOF. Let Q be one of the linear optimal rules in Theorem 2.1.4, and take $\varepsilon \in [-1, 1]$. Then

$$\hat{Q}[\varepsilon f] - Q[\varepsilon f] \le \rho^{\text{opt}} = \hat{Q}[0];$$

that is,

$$\hat{Q}[\varepsilon f] - \hat{Q}[0] \le \varepsilon Q[f]$$

and therefore

$$\lim_{\varepsilon \downarrow 0} \frac{\hat{Q}[\varepsilon f] - \hat{Q}[0]}{\varepsilon} \le Q[f], \qquad \lim_{\varepsilon \uparrow 0} \frac{\hat{Q}[\varepsilon f] - \hat{Q}[0]}{\varepsilon} \ge Q[f].$$

These limits exist because concave functions have one-sided derivatives; if they coincide for each $f \in \mathcal{C}$, then they must both be equal to $Q[f]$ and the uniqueness of the optimal rule is proved.

Note that

$$\frac{\hat{Q}[\varepsilon f] - \hat{Q}[0]}{\varepsilon} = \frac{Q^{\text{so}}[\varepsilon f]}{\varepsilon} + \frac{\rho^{\text{intr}}[\varepsilon f] - \rho^{\text{intr}}[0]}{\varepsilon}.$$

Thus, the theorem follows if we can prove the existence of

$$\lim_{\varepsilon\to 0}\frac{Q^{\rm so}[\varepsilon f]}{\varepsilon}. \tag{2.16}$$

The existence of this limit is a consequence of

$$\begin{aligned}\frac{Q^{\rm so}[\varepsilon f]}{\varepsilon} &= \frac{1}{2}\left(\frac{\hat{Q}[\varepsilon f]-\hat{Q}[0]}{\varepsilon}+\frac{\check{Q}[\varepsilon f]+\hat{Q}[0]}{\varepsilon}\right)\\ &= \frac{1}{2}\left(\frac{\hat{Q}[\varepsilon f]-\hat{Q}[0]}{\varepsilon}+\frac{\hat{Q}[-\varepsilon f]-\hat{Q}[0]}{-\varepsilon}\right).\end{aligned}$$

As above, we see that the one-sided limit as $\varepsilon\downarrow 0$ of the right-hand side exists. The other one-sided limit, as $\varepsilon\uparrow 0$, is obtained by exchanging the two summands in brackets and using equation (2.1). This proves the existence of (2.16). □

EXAMPLE 2.1.2 (continued). By using the explicit formulas for $Q^{\rm so}$ and $\rho^{\rm intr}$ given in (2.11) and (2.12), the limits in Theorem 2.1.5 can easily be calculated, giving us the unique linear optimal rule

$$Q^{\rm opt}[f]=\frac{\sqrt{2}}{4}f(-1)+\left(2-\frac{\sqrt{2}}{2}\right)f(0)+\frac{\sqrt{2}}{4}f(1), \tag{2.17}$$

which is simpler than $Q^{\rm so}$. However, the optimal formula can be much worse than strongly optimal in the sense that

$$\sup_{f\in\mathcal{C}}\frac{I[f]-Q^{\rm opt}[f]}{\rho^{\rm intr}[f]}=\infty. \tag{2.18}$$

This can be seen, for instance, by considering $f(x)=Mx^2/2$.

Let us mention a further aspect relating to linear rules. For fixed $f\in\mathcal{C}$ and any $Q\in\mathbf{Q}^{\rm gen}$, the "uncertainty interval"

$$\bigl[Q[f]-\rho(Q),\, Q[f]+\rho[Q]\bigr]$$

contains the exact value $I[f]$. We can reduce the uncertainty by intersecting intervals associated with different estimation rules. Theorem 2.1.2 implies that the smallest possible uncertainty interval, $I[\mathrm{Info}(f)]=\bigl[\check{Q}[f],\,\hat{Q}[f]\bigr]$, is the intersection of all the uncertainty intervals associated with *linear* rules.

EXAMPLE 2.1.3. Suppose that we are given the function values $f(-1)=0$, $f(0)=0$ and $f(1)=3/2$ together with the information $\sup_{-1\le x\le 1}|f''(x)|\le 2$. These conditions are satisfied by $f(x)=3(x^2+x)/4$, for example. What can we say about $\int_{-1}^{1}f(x)\,dx$?. Example 2.1.2 gives a complete answer: the value of the integral is contained in the interval

$$\left[\frac{7\sqrt{14}-16}{24},\,\frac{16-\sqrt{2}}{24}\right]=[0.424\ldots,\,0.607\ldots], \tag{2.19}$$

and no better result is possible. If we do not know $Q^{\rm so}$ (as is the case in almost all real-world problems), then we have to use another estimation rule, preferably an optimal one. Using (2.13) and (2.17), we obtain the uncertainty interval

$$\left[\frac{17\sqrt{2}-16}{24},\ \frac{16+\sqrt{2}}{24}\right] = [0.335\ldots,\ 0.725\ldots].$$

If we were to use the trapezoidal rule (see Example 2.1.1), we would obtain $Q_3^{\rm Tr}[f] = 3/4$. This is remarkable, for (2.19) shows that there is no function from Info$[f]$ with this integral. The interval of uncertainty is now

$$\left[\frac{5}{12},\ \frac{13}{12}\right] = [0.416\ldots,\ 1.083\ldots]$$

(here we have used $\rho(Q_{n+1}^{\rm Tr}) = (b-a)^3M/(12n^2)$ in the SEF with $\mathcal{C} = \mathcal{C}_M^{(2)}$). Another frequently used rule is Simpson's rule

$$Q_3^{\rm Si}[f] := \frac{1}{3}\big[f(-1) + 4f(0) + f(1)\big]$$

(see Examples 2.2.1 and 4.3.1), which gives the uncertainty interval

$$\left[\frac{49}{162},\ \frac{113}{162}\right] = [0.302\ldots,\ 0.697\ldots].$$

Observe that intersection of the last two intervals, which were obtained from very simple and popular rules, leads to a better result than application of the sophisticated rule (2.17). Examples like this show that one should be wary of putting too much faith in optimal rules.

2.2. Linear rules that are exact on a subspace

As a consequence of Smolyak's theorem (Theorem 2.1.4), from now on we will consider linear estimation rules only. We shall continue to take a fixed SEF as our basis.

In nearly all practical contexts, large analytical problems arise in the course of calculating optimal rules; see, for example, Köhler (1988a), in which a simple and natural SEF is considered. Ever since the early stages of the development of quadrature theory, another principle has been used, which is based on the expectation that an estimation rule that produces the correct value for elements from a particular subspace is likely to give a good approximation for all elements of V. Before giving a formal statement of the principle, we need a definition.

Definition 2.2.1. The linear functional

$$R := I - Q$$

is called the *remainder* of the estimation rule $Q \in \mathbf{Q}$.

Basic Principle. *Choose a subspace $U \subset V$ and find $Q \in \mathbf{Q}$ such that*

$$R[U] = \{0\}. \tag{2.20}$$

Equation (2.20) means that Q is "exact on U". In quadrature theory, U is typically chosen to be a space of polynomials (Chapter 5), trigonometric polynomials

(Chapter 8), natural spline functions (Section 4.7), other types of splines (Theorem 3.3.4, Example 3.3.1 and Theorem 7.3.2), other piecewise polynomials (see (7.31) and Section 7.4), rational functions (Example 2.3.2) or general Chebyshev systems (Section 3.4).

We may not prescribe arbitrary subspaces U; in a permissible subspace, the functional I that we want to calculate has to be linearly dependent on the observation functionals. An alternative formulation of the principle is given by the following theorem.

THEOREM 2.2.1. There is a $Q \in \mathbf{Q}$ satisfying equation (2.20) if and only if

$$I[U \cap \operatorname{Ker} O] = \{0\}. \tag{2.21}$$

PROOF. (i) If Q satisfies equation (2.20), then

$$I[U \cap \operatorname{Ker} O] = Q[U \cap \operatorname{Ker} O] = \{0\}.$$

(ii) Conversely, suppose that (2.21) holds. Let $\{O[u_i] : i = 1, \ldots, m\}$ be a basis of $O[U]$ and let $U_0 := \operatorname{span}\{u_1, \ldots, u_m\}$. Define a linear map A on $O[U]$ by

$$AO[u_i] = I[u_i] \quad \text{for } i = 1, \ldots, m$$

and, if $m < n$, extend it to $\mathbb{R}^n$. Then the estimation rule $Q := AO$ satisfies $R[U_0] = \{0\}$. Take an arbitrary $u \in U$; then there exists $u_0 \in U_0$ such that $O[u] = O[u_0]$. Therefore

$$R[u] = R[u - u_0] = I[u - u_0] - Q[u - u_0] = 0 - 0 = 0$$

and (2.20) is established. □

It seems natural to consider spaces U in (2.20) that are of dimension $\dim U = n$, since we have n degrees of freedom in the choice of Q, i.e. in the linear map $A : \mathbb{R}^n \to \mathbb{R}$ defining Q ($= AO$). The following well-known result from linear algebra is useful.

LEMMA 2.2.1. Let U be a subspace of V with $\dim U = n$. Then the following statements are equivalent:

(2.22) $U \cap \operatorname{Ker} O = \{0\}$.

(2.23) $\dim O[U] = n$.

(2.24) For each $x \in \mathbb{R}^n$, there exists $u \in U$ satisfying $O[u] = x$.

Using this lemma, we obtain the following theorem.

THEOREM 2.2.2. Let U be an n-dimensional subspace of V that satisfies (one of) the equivalent conditions of Lemma 2.2.1. Then there exists exactly one $Q \in \mathbf{Q}$ that has property (2.20).

PROOF. Since U is n-dimensional, any $n+1$ linear functionals must be linearly dependent in U. The preceding lemma tells us that the components of O are linearly independent. Therefore I has to be a linear combination of the components of O; that is, $I = AO$ on U for a certain unique A. □

DEFINITION 2.2.2. The estimation rule Q in Theorem 2.2.2 is called a *projection rule corresponding to U*.

This designation is explained by the following result.

THEOREM 2.2.3. Suppose that the assumptions of Theorem 2.2.2 are satisfied. Then the resulting estimation rule has the representation

$$Q = I \circ P$$

where P is a projection (i.e. a linear map defined on V that satisfies $P \circ P = P$) onto U with

$$O \circ P = O. \tag{2.25}$$

This projection is defined uniquely by U and (2.25).

PROOF. According to Lemma 2.2.1, the restriction of O to U is regular, so that

$$P := \left(O\big|_U\right)^{-1} \circ O$$

is defined. One can readily verify that P is a projection and that (2.25) holds. From the definition of P, it follows that $I \circ P \in \mathbf{Q}$. The projection property means that

$$Q[u] = (I \circ P)[u] = I[u] \quad \text{for all } u \in U.$$

Now let P_1 be another projection that satisfies (2.25). Then

$$O\big(P[f] - P_1[f]\big) = 0 \quad \text{for all } f \in V$$

and the lemma yields $P = P_1$. □

Taking $V = C[a,b]$ and $O[f] = \big(f(x_1), \dots, f(x_n)\big)$, equation (2.25) becomes

$$P[f](x_i) = f(x_i) \quad \text{for } i = 1, \dots, n.$$

This is an interpolation property, and Theorem 2.2.3 says, for instance, that the exactness for $\mathbb{P}_{n-1}$ can be obtained by applying I to the interpolation polynomial.

EXAMPLE 2.2.1. Let

$$V = C[a,b], \qquad I[f] = \int_a^b f(x)\,dx, \qquad O[f] = \Big(f(a), f\big((a+b)/2\big), f(b)\Big).$$

Let $\mathcal{C}$ be arbitrary and take $U = \mathbb{P}_2$. Each $Q \in \mathbf{Q}$ has the form

$$Q[f] = a_1 f(a) + a_2 f\left(\frac{a+b}{2}\right) + a_3 f(b).$$

Upon choosing basis elements $u_i \in \mathbb{P}_2$ given by $u_i(x) = x^i$, equation (2.20) reads

$$\begin{array}{ccccccc} a_1 & + & a_2 & + & a_3 & = & b - a\,, \\ a_1 a & + & a_2\left(\dfrac{a+b}{2}\right) & + & a_3 b & = & \dfrac{b^2 - a^2}{2}\,, \\ a_1 a^2 & + & a_2\left(\dfrac{a+b}{2}\right)^2 & + & a_3 b^2 & = & \dfrac{b^3 - a^3}{3}\,. \end{array}$$

The solution yields Simpson's rule

$$Q_3^{\mathrm{Si}}[f] = \frac{b-a}{6}\left[f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right]. \tag{2.26}$$

On the other hand, the projection P from Theorem 2.2.3 is given by

$$P[f](x) = \frac{2}{(b-a)^2}\Bigg[f(a)\left(x-\frac{a+b}{2}\right)(x-b) - 2f\left(\frac{a+b}{2}\right)(x-a)(x-b) + f(b)(x-a)\left(x-\frac{a+b}{2}\right)\Bigg]. \tag{2.27}$$

Application of the functional I, i.e. integration, again yields the rule (2.26).

Theorem 2.2.1 shows that, moreover, Simpson's rule satisfies $R[\mathbb{P}_3] = \{0\}$, since

$$\int_a^b (x-a)\left(x-\frac{a+b}{2}\right)(x-b)\,dx = 0.$$

A projection P is said to be *based on* O if there exists a factorization $P = L \circ O$ for some map L. Not every $Q \in \mathbf{Q}$ that is exact on U (where $\dim U = n$) can be represented in the form $I \circ P$ with P being a projection onto U based on O. If $U \cap \operatorname{Ker} O \neq \{0\}$, then there is no such projection.

Example 2.2.2. Let

$$V = C[0, 2\pi], \qquad I[f] = \int_0^{2\pi} f(x)\,dx,$$

$$O[f] = \big(f(x_1), f(x_2), \dots, f(x_{2m})\big), \qquad x_\nu = \left(\nu - \tfrac{1}{2}\right)\frac{\pi}{m}$$

and

$$U = \operatorname{span}\{1,\ \cos x,\ \cos 2x, \dots,\ \cos mx,\ \sin x,\ \sin 2x, \dots,\ \sin\,(m-1)x\}.$$

Equation (2.22) is not satisfied, as $u_0(x) = \cos mx$ shows; hence there is no projection rule corresponding to U. Nevertheless, Q_{2m}^{Mi} is exact for U. This follows from the fact that

$$\sum_{\nu=1}^{2m} e^{ikx_\nu} = e^{ik\pi/(2m)} \sum_{\nu=0}^{2m-1} e^{i\nu k\pi/m} = e^{ik\pi/(2m)}\,\frac{e^{i2k\pi}-1}{e^{ik\pi/m}-1} = 0$$

for $k = 1, 2, \dots, 2m-1$, upon separating the real and imaginary parts.

It is possible to prove that $U \cap \operatorname{Ker} O = \operatorname{span}\{u_0\}$, so that the existence of a rule which is exact for U would be a consequence of Theorem 2.2.1, but the proof given above leads to a more complete result.

The advantage of constructions obtained via application of (2.20) is that we need only solve a system of linear equations for the coefficients of A in $Q = AO$. We are free to use any U in (2.21), but evidently we would do better by taking the co-observation into account. It seems natural to quantify the disadvantage of applying an arbitrary rule Q by comparing its error with that of the optimal rule, so we define

$$\operatorname{loss}(Q) := \frac{\rho(Q)}{\rho^{\mathrm{opt}}}.$$

Ideally, we would like to combine easy constructibility with small loss. The realization of this ideal is embodied in the concept of reconstruction.

DEFINITION 2.2.3. A projection P based on O from V onto $U \subset V$ is called a *reconstruction* if

$$P[f] \in \operatorname{Info}(O[f]) \quad \text{for all } f \in \mathcal{C}. \tag{2.28}$$

THEOREM 2.2.4. For a reconstruction P,

$$\big|I[f] - I \circ P[f]\big| \le 2\rho^{\text{intr}}[f]\,. \tag{2.29}$$

PROOF. $I \circ P$ is an estimation rule. Furthermore, we have

$$\check{Q}[f] - \hat{Q}[f] \le I[f] - (I \circ P)[f] \le \hat{Q}[f] - \check{Q}[f]$$

and so the assertion is proved. □

EXAMPLE 2.2.3. We use the SEF of Example 2.2.1 specified by

$$\mathcal{C} = \{f \,:\, f'' \text{ is continuous and } \sup_{x\in[a,b]} |f''(x)| \le M\}.$$

The projection (2.27) is then a reconstruction, since $O \circ P = O$ is obvious and

$$\big(P[f]\big)''(x) = \frac{4}{(b-a)^2}\left[f(a) - 2f\left(\frac{a+b}{2}\right) + f(b)\right] = f''(\xi) \quad \text{for } \xi \in [a,b].$$

The resulting inequality

$$\sup_{f\in\mathcal{C}} \left|\frac{I[f] - Q^{\text{Si}}[f]}{\rho^{\text{intr}}[f]}\right| \le 2 \tag{2.30}$$

demonstrates a certain superiority of Simpson's rule over the optimal rule, since the corresponding left-hand side of (2.30) for the optimal rule is unbounded; see (2.18). This unboundedness holds for all linear estimation rules apart from Q^{Si}.

Unfortunately, there are only few cases where an SEF allows reconstruction. Hence, the elegant method of Theorem 2.2.4 is rarely applicable. A less restrictive notion is that of a δ-reconstruction.

DEFINITION 2.2.4. A projection P based on O onto $U \subset V$ is called a δ-*reconstruction* if for all $f \in \mathcal{C}$ we have:

(i) $P[f] \in \delta\mathcal{C}$ ($:= \{\delta f \,:\, f \in \mathcal{C}\}$);
(ii) $OP[f] = O[f]$.

THEOREM 2.2.5. A δ-reconstruction P satisfies

$$\big|I[f] - I \circ P[f]\big| \le (1+\delta)\rho^{\text{opt}}[f]. \tag{2.31}$$

PROOF. We have

$$\frac{f - P[f]}{\delta + 1} \in \mathcal{C},$$

and an application of Theorem 2.1.1 gives

$$\begin{aligned}
\big|I[f] - (I \circ P)[f]\big| &= \big|I[f - P[f]]\big| \\
&\le (\delta+1)\sup\{I[g] \,:\, g \in \mathcal{C} \cap \operatorname{Ker} O\} \\
&= (\delta+1)\rho^{\text{opt}}
\end{aligned}$$

as claimed. □

Note that (δ-)reconstructions are independent of the functional I under consideration. If we have a reconstruction, then we can use any linear functional and always obtain a good method in the sense of (2.29) or (2.31). In particular, we have $\text{loss}(I \circ P) \leq 2$ for reconstructions and $\text{loss}(I \circ P) \leq 1 + \delta$ for δ-reconstructions.

Examples of δ-reconstructions can be found in the following works: Brass (1995b) for quadratic and cubic splines, Brass (1996) for periodic splines, and Fischer (1997) for trigonometric polynomials.

2.3. Strong optimality: inner product spaces

We return to the construction of strongly optimal rules Q^{so}; the construction will be done according to the principle based on (2.20). An appropriate subspace U has to be chosen such that the resulting estimation rule is strongly optimal. This is not possible for an arbitrary SEF since, in general, Q^{so} is nonlinear (see, e.g., Brass 1998a). Golomb and Weinberger (1959) showed by means of an elegant theory that such a choice is possible if $\mathcal{C}$ is a ball in a Hilbert space.

We need something slightly weaker than a Hilbert space.

Definition 2.3.1. An SEF will be called an *inner product SEF* if:

- a semi-definite inner product $\varphi(\cdot\,,\cdot)$ is defined on V;
- the co-observation is given by
$$\mathcal{C} = \{f \in V : \varphi(f,f) \leq M^2\} \quad \text{for some } M > 0;$$
- the observation O satisfies

$$\{f \in V : \varphi(f,f) = 0\} \cap \operatorname{Ker} O = \{0\}. \tag{2.32}$$

The key step is the choice of an appropriate subspace into which we want to project.

Definition 2.3.2. A space

$$S := (\operatorname{Ker} O)^{\perp} \big(:= \{s \in V : \varphi(g,s) = 0 \text{ for all } g \in \operatorname{Ker} O\}\big) \tag{2.33}$$

of dimension n is called a *spline space* for V and O.

Note that $s \in S \cap \operatorname{Ker} O = (\operatorname{Ker} O)^{\perp} \cap \operatorname{Ker} O$ implies $\varphi(s,s) = 0$, and (2.32) then shows that $s = 0$. Hence, by Theorems 2.2.2 and 2.2.3, we may project into spline spaces.

We furthermore introduce a semi-norm $\|\cdot\|$, defined by

$$\|f\| := \varphi(f,f)^{1/2}.$$

The next theorem says that in an inner product SEF, the projection rule corresponding to the spline space is always strongly optimal. This result is independent of the linear functional under consideration.

Theorem 2.3.1 (Golomb and Weinberger 1959). In an inner product SEF with spline space S, the strongly optimal rule Q^{so} is the unique linear estimation rule such that

$$R[S] = \{0\}.$$

(where R is the remainder). It can be written as

$$Q^{\text{so}} = I \circ P,$$

where P is the projection onto S satisfying

$$O \circ P = O.$$

Moreover, P is an orthogonal projection, i.e.

$$\varphi(f - P[f], s) = 0 \quad \text{for all } f \in V \text{ and } s \in S, \tag{2.34}$$

and furthermore

$$\rho^{\text{intr}}[f] = \left(1 - \frac{\|P[f]\|^2}{M^2}\right)^{1/2} \rho^{\text{opt}}. \tag{2.35}$$

Proof. For the projection P onto S (which exists), equation (2.34) holds since $f - P[f] \in \operatorname{Ker} O$ and $S \perp \operatorname{Ker} O$.

We have to prove strong optimality of the projection rule. Define the set W by

$$\operatorname{Info}[f] = P[f] + W.$$

Then

$$\begin{aligned} W &= \{w \in \operatorname{Ker} O : \|w + P[f]\|^2 \ (= \|w\|^2 + \|P[f]\|^2) \ \le M^2\} \\ &= \{w \in \operatorname{Ker} O : \|w\|^2 \le M^2 - \|P[f]\|^2\}, \end{aligned}$$

and so

$$\begin{aligned} \hat{Q}[f] &= (I \circ P)[f] + \sup\{I[w] : w \in W\} \\ &= IP[f] + \left(\frac{M^2 - \|P[f]\|^2}{M^2}\right)^{1/2} \sup\{I[v] : v \in \mathcal{C} \cap \operatorname{Ker} O\}. \end{aligned}$$

Equation (2.1) yields $\check{Q}[f]$ and hence the strong optimality of $I \circ P$. Now, equation (2.35) follows from Theorem 2.1.1. □

Example 2.3.1. Let V be the space of all continuous and piecewise continuously differentiable functions on $[a, b]$, and define an inner product on V by

$$\varphi(f, g) := \int_a^b f'(x) g'(x)\, dx.$$

Furthermore, let $I[f] = \int_a^b f(x)\, dx$, $O[f] = \big(f(x_1), \ldots, f(x_n)\big)$ for $a \le x_1 < x_2 < \cdots < x_n \le b$, and

$$\mathcal{C} = \left\{ f : \int_a^b [f'(x)]^2\, dx \le M^2 \right\}.$$

We have

$$|f(x) - f(x_1)| = \left| \int_{x_1}^x f'(u)\, du \right| \le \left(|x - x_1| \int_{x_1}^x \left[f'(u)\right]^2 du \right)^{1/2} \le M|b - a|^{1/2}.$$

Therefore $|f - f(x_1)|$ is uniformly bounded for all $f \in \mathcal{C}$, so that $\hat{Q} - \check{Q}$ is uniformly bounded. If $\varphi(f, f) = 0$, this bound is zero and $O[f] = 0$ implies, in particular, that $f(x_1) = 0$. Hence, equation (2.32) holds and we have an inner product SEF.

The corresponding spline space is the space of "natural spline functions of order one", i.e. the space of polygonal lines with vertices at $x_1, \ldots, x_n$ which are constant on $[a, x_1]$ and on $[x_n, b]$. Integration by parts shows that for each such natural spline s, $\varphi(f, s) = \int_a^b f'(x) s'(x)\, dx$ is a linear combination of $f(x_1), \ldots, f(x_n)$. We thus obtain $s \in (\operatorname{Ker} O)^\perp$. Obviously, for each $(y_1, \ldots, y_n) \in \mathbb{R}^n$ we can find an

$s \in S$ satisfying $s(x_i) = y_i$. Hence we have $\dim S = n$, and Theorem 2.3.1 is applicable. The projected element $P[f]$ is the natural spline function of order one that interpolates f at $x_1, \ldots, x_n$. Using simple geometric arguments, one can show that Q^{so} is the generalized trapezoidal rule in Example 2.1.1. Formula (2.35) reads as follows:

$$\rho^{\text{intr}}[f] = \left(1 - \sum_{\nu=1}^{n-1} \frac{[f(x_{\nu+1}) - f(x_\nu)]^2}{M^2(x_{\nu+1} - x_\nu)}\right)^{1/2} \rho^{\text{opt}},$$

where ρ^{opt} can be determined via Peano kernel methods (see Section 4.2). Here we just note the result:

$$\rho^{\text{opt}} = M\left(\frac{(x_1 - a)^3}{3} + \frac{1}{12}\sum_{\nu=1}^{n-1}(x_{\nu+1} - x_\nu)^3 + \frac{(b - x_n)^3}{3}\right)^{1/2}.$$

In many situations in numerical analysis, a small norm indicates good quality. A nice property that projections into spline spaces have is that they map onto the interpolating elements of minimal semi-norm ("interpolating" means having the same observation).

THEOREM 2.3.2. Under the assumptions of Theorem 2.3.1, for any $f, g \in V$ such that $O[g] = O[f]$ we have

$$\|g\| \geq \|P[f]\|,$$

with equality holding if and only if $g = P[f]$.

PROOF. Let $O[g] = O[f]$, i.e. $g - P[f] \in \operatorname{Ker} O$, and let $P[f] \in S$. It follows that

$$\begin{aligned} \|g\|^2 &= \|P[f] + g - P[f]\|^2 \\ &= \|P[f]\|^2 + 2\underbrace{\varphi(P[f],\, g - P[f])}_{=0} + \|g - P[f]\|^2 \geq \|P[f]\|^2. \end{aligned}$$

Equality holds if and only if $\|g - P[f]\| = 0$, i.e. if $g = P[f]$ (see the assumption (2.32)). ☐

Thus, the interpolating spline function from Example 2.3.1 is the "flattest" interpolating element in the sense that among all the $g \in V$ which interpolate f at $x_1, \ldots, x_n$, the minimal value of

$$\|g'\|_2^2 = \int_a^b \left[g'(x)\right]^2 dx$$

is attained by $g = P[f]$.

We will now strengthen our assumptions on V by requiring V to be a Hilbert space. A new tool, namely the Riesz representation theorem (see any text on functional analysis), now becomes available to us.

Riesz Representation Theorem. *Suppose l is a continuous linear functional on a Hilbert space V; then there exists one and only one $\widetilde{l} \in V$ (called the representer of l) such that*

$$l(x) = \varphi(x, \widetilde{l}) \quad \textit{for all } x \in V.$$

Furthermore,

$$\|l\| = \|\widetilde{l}\|.$$

An immediate consequence of this theorem is the following result.

THEOREM 2.3.3. Let V be a Hilbert space and let $o_1, \ldots, o_n$ be continuous and linearly independent functionals. Then a spline space for V and $O = (o_1, \ldots, o_n)$ is given by $\mathrm{span}(\widetilde{o}_1, \ldots, \widetilde{o}_n)$.

The spaces V of greatest relevance to us consist of real-valued functions f defined on $X \subset \mathbb{R}^d$. In such spaces we can define functionals l_y by

$$l_y[f] := f(y) \quad \text{for } y \in X.$$

If these functionals l_y are continuous, the Riesz representation theorem implies the existence of a function $K(\cdot\,,\cdot)$ on $X \times X$ such that

$$f(y) = \varphi(f, K(\cdot, y)) \quad \text{for } f \in V,\ y \in X.$$

This function K is called the *reproducing kernel*. Determination of the reproducing kernel is made simpler if an orthonormal basis of H is available, i.e. a sequence $u_i \in H,\ i = 1, 2, \ldots,$ with

$$f = \sum_{i=1}^{\infty} \varphi(u_i, f) u_i \quad \text{for all } f \in H.$$

We then have

$$K(x, y) = \sum_{i=1}^{\infty} u_i(x) u_i(y) \quad \text{for } x, y \in X,$$

and from this we easily deduce that

$$\widetilde{l}(y) = l[K(\cdot, y)]$$

for all continuous linear functionals on spaces of the aforementioned type. For more information on the theory of reproducing kernels, see Meschkowski (1962). We now illustrate the theory by an example.

EXAMPLE 2.3.2. Fix $\rho > 0$, and let $p_\nu(x) = x^\nu$,

$$\mathcal{H}_\rho = \Big\{ f : f = \sum_{\nu=0}^{\infty} \alpha_\nu p_\nu \text{ with } \alpha_\nu \in \mathbb{R} \text{ and } \sum_{\nu=0}^{\infty} \alpha_\nu^2 \rho^{2\nu} < \infty \Big\}$$

and

$$\varphi\Big(\sum_{\nu=0}^{\infty} \alpha_\nu p_\nu\,,\ \sum_{\nu=0}^{\infty} \beta_\nu p_\nu \Big) = \sum_{\nu=0}^{\infty} \alpha_\nu \beta_\nu \rho^{2\nu}.$$

Evidently, $\mathcal{H}_\rho$ is a Hilbert space of holomorphic functions, and

$$u_i(x) = x^i \rho^{-i} \quad \text{for } i = 0, 1, \ldots$$

is an orthonormal basis for $\mathcal{H}_\rho$. Hence

$$K(x, y) = \sum_{i=0}^{\infty} x^i y^i \rho^{-2i} = \frac{\rho^2}{\rho^2 - xy}$$

is the reproducing kernel, and the spline space for $O[f] = (f(x_1), \ldots, f(x_n))$ is $S = \mathrm{span}\{K(x_i, y) : i = 1, \ldots, n\}$. Projecting onto S means interpolating, and we can construct $P[f]$. By analogy with the Lagrange interpolation formula, the interpolant can be written in the form

$$P[f](x) = \sum_{\lambda=1}^{n} f(x_\lambda) \frac{z(x)}{(x - x_\lambda) z'(x_\lambda)} \cdot \frac{v(x_\lambda)}{v(x)}$$

$$\text{where} \qquad z(x) = \prod_{\nu=1}^{n} (x - x_\nu), \qquad v(x) = \prod_{\nu=1}^{n} (\rho^2 - x x_\nu).$$

Now, $I \circ P$ is the strongly optimal rule. In the special case where $I[f] = \int_{-1}^{1} f(u)du$ and $\rho > 1$, we can obtain (by expanding in partial fractions) a fairly explicit expression

$$Q^{\mathrm{so}}[f] = \sum_{\nu=1}^{n} a_\nu f(x_\nu)$$

$$\text{where} \qquad a_\lambda = \rho^{-2n+2} \sum_{\kappa=1}^{n} \frac{v(x_\kappa) v(x_\lambda)}{z'(x_\kappa) z'(x_\lambda)} \cdot \frac{1}{\rho^2 - x_\kappa x_\lambda} \cdot \frac{1}{x_\kappa} \ln \frac{\rho^2 + x_\kappa}{\rho^2 - x_\kappa};$$

see Wilf (1967) and Valentin (1968). For the determination of best nodes, see Engels (1977).

Further examples of how the theory presented in this section can be applied are given in Barnhill (1967, 1968), Rabinowitz and Richter (1970a, 1970b) and Chawla and Raina (1972).

As mentioned before, the availability of an orthonormal basis $u_1, u_2, \ldots$ for the underlying Hilbert space often simplifies things considerably. The following theorem is further evidence of this.

THEOREM 2.3.4. Let Q be any estimation rule in a given Hilbert space SEF. Then

$$\rho(Q) = M \left[\sum_{i=1}^{\infty} \big(R[u_i]\big)^2 \right]^{1/2}.$$

PROOF. We apply Parseval's equation

$$\varphi(f, f) = \sum_{i=1}^{\infty} \varphi^2(f, u_i)$$

(which holds for any f from the Hilbert space and is an easy consequence of the definitions) to $f = \widetilde{R}$. This gives

$$\begin{aligned} \rho(Q) &= \sup\{R[f] : \varphi(f, f) \le M^2\} = M\|R\| = M\|\widetilde{R}\| = M\big[\varphi(\widetilde{R}, \widetilde{R})\big]^{1/2} \\ &= M \left[\sum_{i=1}^{\infty} \varphi^2(\widetilde{R}, u_i) \right]^{1/2} = M \left[\sum_{i=1}^{\infty} \big(R[u_i]\big)^2 \right]^{1/2} \end{aligned}$$

as claimed. $\square$

The formula

$$\rho(Q) = M \left(\sum_{i=1}^{\infty} \big(I[u_i] - Q[u_i]\big)^2 \right)^{1/2}$$

leads to an apparently new principle for the construction of estimation rules, namely: for a given Hilbert space SEF, choose $Q \in \mathbf{Q}$ such that

$$\sum_{i=1}^{\infty} \big[I[u_i] - Q[u_i]\big]^2$$

is as small as possible; see Wilf (1964). The minimum, however, is ρ^{opt}, and it is attained by a rule that can be constructed using our basic principle of requiring exactness on a suitable subspace.

2.4. Varying the observation

We wish to generalize our model so that we are not restricted to assuming a fixed observation. Instead, our approach will be to take a (large) set of observations and try to choose one that is appropriate for the particular estimation problem at hand.

DEFINITION 2.4.1. A *generalized SEF* is a quadruple $(V, I, \Omega, \mathcal{C})$ where V, I and $\mathcal{C}$ are as in the definition of a SEF (Definition 2.1.1) and Ω is a set of linear functionals on V.

In this section we shall always assume a generalized SEF.

For any $O \in \Omega^n$, the quadruple $(V, I, O, \mathcal{C})$ is an SEF. All notions from the previous sections can be used here, if the additional dependence on O is included; for example, we now write $\rho^{\text{opt}}(O)$ or $\mathbf{Q}(O)$.

DEFINITION 2.4.2. Define $\rho_n^{\text{best}} := \inf\{\rho^{\text{opt}}(O) \,:\, O \in \Omega^n\}$.
Then $Q_n^{\text{best}} := Q \in \bigcup\limits_{O\in\Omega^n} \mathbf{Q}(O)$ is called a *best estimation rule* if $\rho(Q) = \rho_n^{\text{best}}$.

EXAMPLE 2.4.1. Consider a generalized SEF given by $V = C[a,b]$, $I[f] = \int_a^b f(x)\,dx$, $\Omega = \{l_x \,:\, x \in [a,b]$ such that $l_x[f] = f(x)\}$ and $\mathcal{C} = \text{Lip}_M 1$. In Example 2.1.1, we determined $\rho^{\text{opt}}(O)$ for arbitrary $O \in \Omega^n$. We thus obtain

$$\begin{aligned} \rho_n^{\text{best}} &= \frac{M}{4}\left\{\inf_{a\le x_1\le x_2\le\ldots\le x_n\le b}\Big(2(x_1-a)^2 + \sum_{\nu=1}^{n-1}(x_{\nu+1}-x_\nu)^2 + 2(b-x_n)^2\Big)\right\} \\ &= \frac{M(b-a)^2}{4n}. \end{aligned}$$

Here, the infimum can be determined with standard methods, and we see that it is attained for $x_\nu = a + (2\nu-1)(b-a)/(2n)$. Hence, the midpoint rule is the best choice in the given generalized SEF.

We know that a precision of $\rho_n^{\text{best}} + \varepsilon$, where $\varepsilon > 0$, can be achieved with a linear rule that is independent of the particular $f \in \mathcal{C}$. Let us now try to improve our results by making a choice of $O \in \Omega^n$ that does take the properties of f into account. In our SEF model, information about the particular $f \in \mathcal{C}$ can be obtained only through $o \in \Omega$; therefore a choice of $O = (o_1, \ldots, o_n) \in \Omega^n$ has to be sequential. This means that, while O is not known *a priori*, the o_i can be chosen based on knowledge of $o_1[f], \ldots, o_{i-1}[f]$.

DEFINITION 2.4.3. An *n-stage sequential* (or *adaptive*) *algorithm* Alg is an algorithm given by:

(i) choice functions $g_i : \Omega^i \times \mathbb{R}^i \to \Omega$ for $i = 1, \dots, n-1$;
(ii) termination functions $h_i : \Omega^i \times \mathbb{R}^i \to \{0, 1\}$ for $i = 1, \dots, n-1$;
(iii) estimation functions $q_i : \Omega^i \times \mathbb{R}^i \to \mathbb{R}$ for $i = 1, \dots, n$;
(iv) a functional $o_1 \in \Omega$.

The application of an n-stage sequential algorithm consists of a number of steps; this number (not more than n) is controlled by the algorithm itself. The final output is an estimate $Q[f]$. We set $g_0 := o_1$ and $h_0 := 0$. The kth step consists of calculating $o_k := g_{k-1}(o_1, \dots, o_{k-1}, o_1[f], \dots, o_{k-1}[f])$, followed by $o_k[f]$ and $h_k(o_1, \dots, o_k, o_1[f], \dots, o_k[f])$. If the latter value is zero, we proceed to the $(k+1)$st step. Otherwise, the process is terminated with the estimate

$$Q[f] = q_k(o_1, \dots, o_k, o_1[f], \dots, o_k[f]).$$

Example 2.4.1 (continued). Define $\widetilde{\Omega} := \{\widetilde{o}_1, \dots, \widetilde{o}_n\}$ where $\widetilde{o}_\nu[f] = f\big(a + (2\nu - 1)(b-a)/(2n)\big)$, and let O_{k-1} be the set of observations that has already been chosen after the $(k-1)$st step. The kth step proceeds as follows. The choice function g_k selects an $o_k \in \widetilde{\Omega} \setminus O_{k-1}$, which is applied to f. Then, $\rho^{\text{intr}}[O_k, f]$ is calculated as in Example 2.1.1. If this number is at most $M(b-a)^2/(4n)$, the termination function h_k is set to 1 and the algorithm terminates with the estimate

$$Q[f] := Q^{\text{so}}[O_k, f].$$

Otherwise, we set h_k to 0 and proceed to the $(k+1)$st step.

Obviously, this algorithm guarantees that

$$\big|I[f] - Q[f]\big| \le \rho_n^{\text{best}} = \frac{M(b-a)^2}{4n}$$

with at most n but often fewer function evaluations. The optimal algorithm from Example 2.4.1 (the earlier part) always requires n function values.

Different selections of the choice functions g_i yield many variants of the algorithm. One can seek to choose g_k so that O_k is always "as equally distributed as possible", or try to "maximize the reduction of the uncertainty" of $I[f]$ in each step. Sukharev (1979) devised an algorithm that is optimal with respect to the necessary number of function evaluations; however, one has to pay for this minimality with choice functions that are quite involved, so it is doubtful that a gain in the overall efficiency of computation can be achieved with Sukharev's algorithm.

To evaluate an algorithm, the quantity

$$\rho(\text{Alg}) := \sup\big\{\big|I[f] - Q[f]\big| \,:\, f \in \mathcal{C}\big\}$$

is crucial. The following remarkable result says, essentially, that "adaptiveness does not help in the worst case".

Theorem 2.4.1 (Bakhvalov 1971). *For each n-stage algorithm Alg, we have*

$$\rho(\text{Alg}) \ge \rho_n^{\text{best}}.$$

Proof. Let $f = 0$ $(\in \mathcal{C})$.

The algorithm chooses the observation $O = (o_1, \dots, o_k)$, where $k \le n$. Application of Theorem 2.1.1 then gives

$$\rho(\text{Alg}) \ge \rho^{\text{intr}}(O, f) = \rho^{\text{intr}}(O, 0) = \rho^{\text{opt}}(O) \ge \inf_{O \in \Omega^k} \rho^{\text{opt}}(O) \ge \rho_n^{\text{best}}$$

as asserted. □

The first result comparing adaptive and non-adaptive algorithms was obtained by Kiefer (1957). For more results in this area, we refer the reader to Gal and Micchelli (1980), Sukharev (1985), Huerta (1986), Sukharev (1987), Novak (1988), Chuyan and Sukharev (1990), and Novak (1992).

Theorem 2.4.1 supplies a further argument for concentrating on linear estimation rules.