

# A best nonlinear quadrature for the Sobolev class $KW^r[a, b]$

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**Abstract** As usual, denote by  $KW^r[a, b]$  the Sobolev class consisting of every function whose  $(r - 1)$ st derivative is absolutely continuous on the interval  $[a, b]$  and its  $r$ th derivative is bounded by  $K$  a.e. in  $[a, b]$ . For a function  $f \in KW^r[a, b]$ , its values and derivatives up to  $r - 1$  order at a set of nodes  $\mathbf{x}$  are known. These values are said to be given Hermite information. This work reports results on best quadrature based on the given Hermite information for the class  $KW^r[a, b]$ . Existence and concrete construction issue of the best quadrature is settled down by perfect spline interpolation. It turns out that the best quadrature depends on a system of algebraic equations satisfied by a set of free nodes of the interpolation perfect spline. From our another new result, it is shown that the system can be converted in a closed form to two single-variable polynomial equations, each being of degree approximately  $r/2$ . It is interesting to mention that the best quadrature and its worst case error bound, although nonlinear in nature, can be recursively expressed in terms of the given Hermite information via combinatorial analysis, obviating solving the nonlinear system. As a by-product, best interpolation formula for the class  $KW^r[a, b]$  is also obtained.

**Keywords:** Sobolev class, Hermite information, perfect spline, optimal recovery, best quadrature.

## 1 Introduction

Let  $r$  be any natural number and  $K$  be any positive number. Let  $C[a, b]$  be the set of all continuous functions defined on an interval  $[a, b]$ . Set

$$KW^r[a, b] = \left\{ f \in C[a, b] \mid f^{(r-1)}(t) \text{ abs. contin.}, |f^{(r)}(t)| \leq K, \text{ a.e. } t \in [a, b] \right\}. \quad (1.1)$$

Write  $W^r := 1W^r[0, 1]$ . Suppose  $\mathbf{x} = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$  is a set of fixed nodes in the interval  $[a, b]$ , satisfying

$$a = x_0 \leq x_1 < x_2 < \dots < x_n \leq x_{n+1} = b.$$

For any  $f \in KW^r[a, b]$ , the following  $r \times n$  matrix

$$\mathcal{H}_{\mathbf{x}}^r(f) := (f^{(j)}(x_i))_{r \times n}, \quad i = 1, 2, \dots, n; \quad j = 0, 1, \dots, r - 1, \quad (1.2)$$

defines a Hermite information operator  $\mathcal{H}_{\mathbf{x}}^r : KW^r[a, b] \rightarrow \mathbb{R}^{r \times n}$  at  $\mathbf{x}$ . When there is only a single node, i.e.,  $\mathbf{x} = (\eta)$ , we write  $\mathcal{H}_{\eta}^r$  instead of  $\mathcal{H}_{(\eta)}^r$ . The Hermite information  $\mathcal{H}_{\mathbf{x}}^r(f)$  is usually expensively obtained from scientific and engineering computing practices, therefore, it is uneconomic or injudicious not to make great utility of thus obtained information. In view of this, the best quadrature formula in the sense of Sard and of Nikolskii seems to be not very suitable for such circumstances since the given information is not fully taken into consideration therein and the following new notion arises more naturally.

Let

$$I(f) := \int_a^b f(t) dt.$$

If  $\bar{f} \in KW^r[a, b]$ , then every formula for approximating the integral  $I(\bar{f})$  can be viewed as a functional acting on  $\mathcal{H}_{\mathbf{x}}^r(KW^r[a, b])$ . Its error bound is defined by

$$E(\mathcal{H}_{\mathbf{x}}^r(f); Q) := \max_{\substack{\bar{f} \in KW^r[a, b] \\ \mathcal{H}_{\mathbf{x}}^r(\bar{f}) = \mathcal{H}_{\mathbf{x}}^r(f)}} |I(\bar{f}) - Q(\mathcal{H}_{\mathbf{x}}^r(f))|.$$

**Definition 1.1.** Among all the quadrature formulae based on the information  $\mathcal{H}_{\mathbf{x}}^r(f) \in \mathcal{H}_{\mathbf{x}}^r(KW^r[a, b])$ , the one  $Q^*(\mathcal{H}_{\mathbf{x}}^r(f))$  which minimizes the error bound

$$E(\mathcal{H}_{\mathbf{x}}^r(f); Q^*) = \min_Q E(\mathcal{H}_{\mathbf{x}}^r(f); Q) =: R(\mathcal{H}_{\mathbf{x}}^r(f))$$

is said to be the best quadrature formula (if it exists) based on the given information  $\mathcal{H}_{\mathbf{x}}^r(f)$ . Correspondingly, the error bound  $R(\mathcal{H}_{\mathbf{x}}^r(f))$  is called the radius of the Hermite information  $\mathcal{H}_{\mathbf{x}}^r(f)$  for the integral  $I(f)$ .

For the given information  $\mathcal{H}_{\mathbf{x}}^r(f) \in \mathcal{H}_{\mathbf{x}}^r(KW^r[a, b])$ , the best quadrature formula in the sense of definition 1.1 is a central algorithm for the integral  $I(\bar{f})$ . It fits into the general framework of optimal recovery theory [1, 2]. Simulating to us are the pioneering works of Kolmogorov [3], Sard [4], Nikolskii [5] and Schoenberg [6] on the study of the best quadrature formulas, however, there is much difference between their notion and our new one. First, the new notion emphasizes that  $\mathcal{H}_{\mathbf{x}}^r(f)$  itself is given. This is unlike the case of optimal recovery theory where the information operator  $\mathcal{H}_{\mathbf{x}}^r$  is given. It is also unlike the cases of Sard [4] (cf. [6]) and of Nikolskii [5], where for the former the nodes  $\mathbf{x}$  are given and for the latter the number of the nodes  $\mathbf{x}$  is given. Second, it is shown here that for the class  $KW^r[a, b]$  the best quadrature formula based on the given information  $\mathcal{H}_{\mathbf{x}}^r(f) \in \mathcal{H}_{\mathbf{x}}^r(KW^r[a, b])$  is in general nonlinear. This stands in vivid contrast against the optimal algorithm, which is guaranteed by the Smolyak theorem [2] to be linear. It is also well-known that the best quadrature formulas both in the sense of Sard and of Nikolskii are linear. One usually obtains them by first representing the error terms by the Peano theorem, using the Hölder inequality and then minimizing the Peano kernel in appropriate senses. Such a linear method do well in the classical cases as in Schoenberg [6] and Nikolskii [7], however, it cannot work in our situation. It should be mentioned that our new notion emphasizes that the Hermite information of the integrand  $\bar{f}$  is already obtained. When considering the errors we need not maximize them in the whole Sobolev class  $KW^r[a, b]$  as in the classical cases, we need only maximize them in the restricted subclass

$$\{\bar{f} \in KW^r[a, b] \mid \mathcal{H}_{\mathbf{x}}^r(\bar{f}) = \mathcal{H}_{\mathbf{x}}^r(f)\}.$$

Certainly, difficulty greatly increases in so doing, but this is another problem. This is the so called making great utility of obtained information mentioned above. Therefore, the error bound for the new best quadrature formula is in general less than that in the sense of Sard. And the latter is realized by the former at the specific information  $\mathcal{H}_{\mathbf{x}}^r(f) = \mathbf{0}$  [1].

To solve the best quadrature formula based on the given Hermite information  $\mathcal{H}_{\mathbf{x}}^r(f) \in \mathcal{H}_{\mathbf{x}}^r(KW^r[a, b])$ , we split the interval  $[a, b]$  into subinterval  $[x_i, x_{i+1}]$ ,  $i = 0, 1, \dots, n$ , and then transform integration interval  $[x_i, x_{i+1}]$  into interval  $[0, 1]$ . By considering perfect spline interpolation over interval  $[0, 1]$ , we find out the extremal functions for  $W^r$ , and hence obtain the best quadrature formula. As a by-product, we settle down the best interpolation problem for  $W^r$ . Transforming thus obtained results to the interval  $[a, b]$  yields our main results.

## 2 Main results

From now on, Let  $e = \pm 1$  and

$$u_-^r = \begin{cases} 0, & \text{if } u \geq 0; \\ u^r, & \text{if } u < 0. \end{cases}$$

Denote  $\Delta x_i = x_{i+1} - x_i$ ,  $i = 0, 1, \dots, n$ , and let  $g[0, 1^j]$  represent the divided difference of a function  $g$  at points 0, 1, where 1 is repeated  $j$  times for any natural number  $j$ . Let  $P_i^r$  be the subset of  $W^r$ , consisting of perfect splines of degree  $r$  which have  $i$  free nodes. Set

$$W_*^r := W^r \setminus \bigcup_{i=0}^{r-1} P_i^r.$$

In what follows, we write  $\mathcal{H}^r := \mathcal{H}_{(0,1)}^r$ .

First, it can be straightforwardly shown that the following lemma concerning perfect spline interpolation problem and the extremal properties of the interpolation perfect spline by an elementary analysis and zero counting argument.

**Lemma 2.1.** Suppose we are given Hermite information  $\mathcal{H}^r(\varphi) \in \mathcal{H}^r(W_*^r)$ . Let the perfect spline of degree  $r$

$$S_{e,r}(t; \varphi) = \sum_{i=0}^{r-1} \frac{\varphi^{(i)}(1)}{i!} (t-1)^i + \frac{e}{r!} \left\{ (1-t)^r - 2 \sum_{i=1}^r (-1)^i (t - \xi_{e,i})^r \right\}, \quad (2.1)$$

satisfy

$$\begin{aligned} 0 < \xi_{e,1} < \dots < \xi_{e,r} < 1, \\ \mathcal{H}^r(S_{e,r}) &= \mathcal{H}^r(\varphi). \end{aligned} \quad (2.2)$$

Then we have

$$\sum_{i=1}^r (-1)^{r-i} \xi_{e,i}^j = \frac{1}{2} (1 - e(-1)^r j! \varphi^{(r-j)}[0, 1^j]), \quad j = 1, \dots, r, \quad (2.3)$$

and

$$S_{-,r}(t) \leq \varphi(t) \leq S_{+,r}(t), \quad t \in [0, 1]. \quad (2.4)$$

As a by-product of Lemma 2.1, we immediately have

**Theorem 2.1.** If  $\mathcal{H}^r(\varphi) \in \mathcal{H}^r(W_*^r)$ , then

$$i_t^*(\mathcal{H}^r(\varphi)) = \frac{S_{+,r}(t) + S_{-,r}(t)}{2}$$

is the unique best interpolation formula which makes the error bound

$$e(\mathcal{H}^r(\varphi); i_t) := \max_{\substack{\varphi \in W_*^r \\ \mathcal{H}^r(\varphi) = \mathcal{H}^r(\varphi)}} |f(t) - i_t(\mathcal{H}^r(\varphi))|$$

attain its minimum

$$e(\mathcal{H}^r(\varphi); i_t^*) = \frac{S_{+,r}(t) - S_{-,r}(t)}{2} = \min_{i_t} e(\mathcal{H}^r(\varphi); i_t) =: r_t(\mathcal{H}^r(\varphi)).$$

Integrating both sides of (2.4) over  $[0, 1]$  respectively produces the best quadrature formula and its information radius based on the given Hermite information  $\mathcal{H}^r(\varphi)$ .

**Theorem 2.2.** The best quadrature formula based on the given Hermite information  $\mathcal{H}^r(\varphi) \in \mathcal{H}^r(W_*^r)$  is

$$Q^*(\mathcal{H}^r(\varphi)) = \sum_{i=1}^r (-1)^{i-1} \frac{\varphi^{(i-1)}(1)}{i!} - \frac{1}{(r+1)!} \sum_{i=1}^r (-1)^{r-i} (\xi_{+,i}^{r+1} - \xi_{-,i}^{r+1}), \quad (2.5)$$

where  $\xi_{e,i}$ ,  $i = 1, \dots, r$ , satisfy (2.3). And its radius of the Hermite information is

$$R(\mathcal{H}^r(\varphi)) = \frac{1}{(r+1)!} \left( 1 - \sum_{i=1}^r (-1)^{r-i} (\xi_{+,i}^{r+1} + \xi_{-,i}^{r+1}) \right). \quad (2.6)$$

Sometimes, the solution of (2.3) can be explicitly found, for example,  $\mathcal{H}^r(\varphi) = \mathbf{0}$ .

**Corollary 2.1.** Let  $\xi_{e,k} = \cos^2 \frac{r+1-k}{2r+2} \pi$ ,  $k = 1, 2, \dots, r$ . Then  $(\xi_{e,1}, \xi_{e,2}, \dots, \xi_{e,r})$  is a solution to the following system of equations

$$\sum_{k=1}^r (-1)^{r-k} \xi_{e,k}^j = \frac{1}{2}, \quad j = 1, \dots, r. \quad (2.7)$$

That is,  $(\xi_{e,1}, \xi_{e,2}, \dots, \xi_{e,r})$  is a solution to the special case of (2.3) corresponding to  $\mathcal{H}^r(\varphi) = \mathbf{0}$ .

A pending problem is that in order to obtain the set of free nodes  $\xi_{e,\nu}$  we have to solve the nonlinear system (2.3) of algebraic equations for every  $e, \nu$ . It is natural to ask whether it is expensive to solve such a system of equations. From the main result in [8] that there holds the next theorem, which states that for fixed  $e, i$  solving the system (2.3) can be in a closed form converted to solving two single-variable polynomial equations, each of whose degrees is no greater than  $r/2$ . This practically guarantees the feasibility of constructing the best quadrature formula.



From this, we derive

**Corollary 2.2.** The best quadrature formula based on the given Hermite information  $\mathcal{H}^2(\varphi) \in \mathcal{H}^2(W_*^2)$  is

$$Q^*(\mathcal{H}^2(\varphi)) = \frac{1}{2}(\varphi(0) + \varphi(1)) + \frac{1}{96}\varphi'[0,1] \left( (\varphi'[0,1])^2 - 9 - \frac{12(\varphi'[0,1] - 2\varphi[0,1^2])^2}{1 - (\varphi'[0,1])^2} \right), \quad (2.13)$$

and its information radius is

$$R(\mathcal{H}^2(\varphi)) = \frac{1}{32} \left( 1 - (\varphi'[0,1])^2 - \frac{4(\varphi'[0,1] - 2\varphi[0,1^2])^2}{1 - (\varphi'[0,1])^2} \right). \quad (2.14)$$

From Corollary 2.2, it not difficult to give the best quadrature formula and its information radius based on the given Hermite information  $\mathcal{H}_x^2(f) \in \mathcal{H}_x^2(KW^2[a, b])$ . That is the main result of [9], see also [10].

But it is really difficult to solve the system (2.3) if  $r$  is large even if we can use Theorem 2.3 to solve two algebraic equations. Sometimes, this kind of matter does not occur thanks to the combinatorial results from [8]. Indeed, from Theorem 2.2, we see that in order to obtain the best quadrature formula and its radius it is equivalent to computing the quantity

$$p_{e,r+1} = \sum_{i=1}^r (-1)^{r-i} \xi_{e,i}^{r+1},$$

for given  $p_{e,1}, p_{e,2}, \dots, p_{e,r}$ . Observe that  $p_{e,r+1}$  depends on  $\xi_{e,1}, \xi_{e,2}, \dots, \xi_{e,r}$ , and thus depends indirectly on  $p_{e,1}, p_{e,2}, \dots, p_{e,r}$ . The following question arises naturally: can we express  $p_{e,r+1}$  in terms of  $p_{e,1}, p_{e,2}, \dots, p_{e,r}$  directly? The answer is yes. From [8], we have the following interesting theorem which says the computation may not resort to solving the nonlinear system (2.3).

**Theorem 2.4.** Suppose that  $\xi_{e,1}, \xi_{e,2}, \dots, \xi_{e,r}$  satisfy the system (2.3). Let  $k = [(r+1)/2]$ , where  $[x]$  denotes the integer part of  $x$ . Then we have

$$p_{e,r+1} = p_{e,r}b_{e,1} - p_{e,r-1}b_{e,2} + \dots + (-1)^{r+1}p_{e,1}b_{e,r} + (-1)^r(r+1)b_{e,r+1}, \quad (2.15)$$

where,

$$b_{e,r+1} := -b_{e,r}a_{e,k+1} - b_{e,r-1}a_{e,k+2} - \dots - b_{e,k+1}a_{e,r}.$$

Here,  $a_{e,k+1}, a_{e,k+2}, \dots, a_{e,r}$  is determined by the following linear system.

$$\begin{pmatrix} b_{e,k+1} \\ b_{e,k+2} \\ \vdots \\ b_{e,r} \end{pmatrix} + \begin{pmatrix} b_{e,k} & b_{e,k-1} & \cdots & b_{e,2k-r+1} \\ b_{e,k+1} & b_{e,k} & \cdots & b_{e,2k-r+2} \\ \vdots & \vdots & & \vdots \\ b_{e,r-1} & b_{e,r-2} & \cdots & b_{e,k} \end{pmatrix} \begin{pmatrix} a_{e,k+1} \\ a_{e,k+2} \\ \vdots \\ a_{e,r} \end{pmatrix} = 0. \quad (2.16)$$

This theorem enables us to write down the best quadrature formula and its radius directly, obviating the need to solve system (2.3) or two algebraic equations (2.8) and (2.9) or (2.10) and (2.11) by Theorem 2.3. For example, the results in Corollary 2.2 can also be obtained via (2.15) and (2.16) after simplification.

Transforming Theorem 2.2 to the interval  $[a, b]$  leads to the following main results.

**Theorem 2.5.** The following formula is the best quadrature formula based on the given Hermite information  $\mathcal{H}_x^r(f) \in \mathcal{H}_x^r(KW^r[a, b])$

$$Q^*(\mathcal{H}_x^r(f)) = \sum_{j=0}^{r-1} (-1)^j \frac{f^{(j)}(x_1)}{(j+1)!} (x_1 - a)^{j+1} + \sum_{i=1}^{n-1} \sum_{j=0}^{r-1} (-1)^j \frac{f^{(j)}(x_{i+1})}{(j+1)!} \Delta x_i^{j+1} - \frac{K}{(r+1)!} \sum_{i=1}^{n-1} \sum_{\nu=1}^r (-1)^{r-\nu} (\xi_{+,i,\nu}^{r+1} - \xi_{-,i,\nu}^{r+1}) \Delta x_i^{r+1} + \sum_{j=0}^{r-1} \frac{f^{(j)}(x_n)}{(j+1)!} (b - x_n)^{j+1}, \quad (2.17)$$

where

$$\sum_{\nu=1}^r (-1)^{r-\nu} \xi_{e,i,\nu}^j = \frac{1}{2} \left( 1 - \frac{e(-1)^r j!}{K} f^{(r-j)}[x_i, x_{i+1}^j] \right), \quad j = 1, \dots, r; \quad i = 1, \dots, n-1, \quad (2.18)$$

and its Hermite information radius for integral is

$$\begin{aligned} R(\mathcal{H}_{\mathbf{x}}^r(f)) &= \frac{K}{(r+1)!} \left\{ (x_1 - a)^{r+1} + \sum_{i=1}^{n-1} \left( 1 - \sum_{\nu=1}^r (-1)^{r-\nu} (\xi_{+,i,\nu}^{r+1} + \xi_{-,i,\nu}^{r+1}) \right) \Delta x_i^{r+1} \right. \\ &\quad \left. + (b - x_n)^{r+1} \right\}. \end{aligned} \quad (2.19)$$

In the spirit of Theorem 2.4,  $Q^*(\mathcal{H}_{\mathbf{x}}^r(f))$  and  $R(\mathcal{H}_{\mathbf{x}}^r(f))$  can also be directly expressed in terms of

$$p_{e,i,j} := \frac{1}{2} \left( 1 - \frac{e(-1)^r j!}{K} f^{(r-j)}[x_i, x_{i+1}^j] \right), \quad j = 1, \dots, r; \quad i = 1, \dots, n-1.$$

The details are left to the interested readers.

Sometimes, the given information

$$\mathcal{H}_{\mathbf{x}}^r(f) = (f^{(j)}(x_i))_{r \times n}, \quad i = 1, 2, \dots, n; \quad j = 0, 1, \dots, r-1,$$

is obtained from scientific computing, we do not know in advance whether it is from the class  $\mathcal{H}_{\mathbf{x}}^r(KW^r[a, b])$ . We also obtain a sufficient and necessary criterion for judging this.

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