On the Power of *a posteriori* Error Estimation for Numerical Integration and Function Approximation

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ABSTRACT

We show that using a type of divided-difference test as an *a posteriori* error criterion, the solutions of a class of simple adaptive algorithms for numerical integration and function approximation such as a piecewise Newton-Cotes rule or a piecewise Lagrange interpolation, are guaranteed to have an approximation-theoretic property of near-optimality. Namely, upon successful termination of the algorithm the solution is guaranteed to be close to the solution given by the spline interpolation method on the same mesh to within any prescribed tolerance.

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1. Introduction

A posteriori estimation, or estimation of truncation error in an algorithm for numerical approximation such as numerical integration, function approximation or solutions of differential equations, is an important part of practical numerical computation. A good *a posteriori* error criterion makes both the algorithm efficient and the solution reliable. This is often achieved through the use of local and adaptive approximations. Namely, in an algorithm, both the approximation and the error estimate are computed locally, and the amount of computation is distributed in the different regions in accordance with the contributions to the total error from these regions as detected by the local error estimates. A good example is an adaptive quadrature for approximating $\int_a^b f(t)\,dt$. In such an algorithm the interval of integration $[a,b]$ is divided into a number of panels and the integral is approximated locally in each panel. The size of a panel and whether it will be further sub-divided both depend on the local error relative to errors in other panels as determined by certain local error checks.

A local, adaptive algorithm of this type has the advantage that in a region where the input function is well-behaved only a small number of panels will be used and so an accurate solution can be obtained with a small computational cost, whereas a region where the input function is "rough" is likely to be detected by a good error estimator and handled with extra care to ensure a satisfactory solution, which sometimes means switching to a special rule for that region. The main disadvantage of these adaptive methods has been their lack of theoretical basis. They have neither known theoretical superiority over non-adaptive methods nor even any approximation-theoretic properties.

The main difficulty that underlies the lack of a theoretical basis is that in solving a numerical approximation problem such as a numerical integration problem the known information during computation is usually incomplete and insufficient to guarantee an error bound. For example, an error estimate for a quadrature approximation relies only on a finite number of computed integrand values, which are not enough to ensure its correctness. Any algorithm can be "fooled" on a well-contrived set of examples.

A traditional theoretical approach to establish the optimality of a numerical quadrature is to show that it is the best in the sense of minimizing the worst-case error on a set of integrands among a class of quadratures. For example, the best quadrature in the sense of Sard (or the optimal quadrature) minimizes the worst-case error for integrands in a bounded subset of a normed function space with certain regularity, among those quadratures which use the same points of function evaluation (or which use the same number of points of function evaluation) (see, e.g., Schoenberg (1969)). In particular, these methods include the spline interpolation methods. However, these quadratures are not being used very often in practice for the reason that they do not have the flexibility for adaptation. They are global methods for which adding new points of function evaluation requires recomputing the whole quadrature including the coefficients. Even though there are theories which say that adaptation has no advantage in the worst-case in this model, it is unrealistic to expect that in practice one can often observe *a priori* the very specific assumptions of the model, i.e., the correct regularity and the correct known bound on a certain higher derivative.

In this paper, we show that, in the case of numerical integration and function approximation, *a posteriori* estimation can bridge this gap between the practice of local, adaptive approximation on the one hand and the theory of optimality enjoyed by some of the global, non-adaptive methods on the other. We present a class of simple *a posteriori* error criteria which, when coupled with simple quadrature formulas, produce adaptive quadrature algorithms whose solutions at termination are guaranteed to possess a property of near-optimality. More specifically, we show that using a type of *a posteriori* divided-difference test and simple local approximation methods such as a Newton-Cotes rule, the solution of an algorithm upon termination is guaranteed to be close to the solution given by the spline interpolation method on the same mesh, to within any prescribed tolerance (Theorem 1). This is despite that, *a priori*, this simple approximation method may not possess any such property. As a corollary, due to the optimality of the spline interpolation method the solution of our algorithm is within the prescribed tolerance to being best *a posteriori* in a sense similar to that of the best quadrature in the sense of Sard (Theorem 2).

Our results also serve as the technical basis for a probabilistic theory of error analysis for the adaptive quadrature algorithms. Theorem 1 is in fact a key lemma for proving that an estimate produced by a modified *a posteriori* error criterion of this type is an upper bound on the conditional expected error of approximation of the quadrature solution given the computed integrand values, under an appropriate assumption of a probability distribution on a set of integrands (Corollary 1). This probabilistic theory (vs. the traditional worst-case theory) was recently developed in Gao (1989) and Gao (1990).

In the following we describe our results in technical terms.

Our setting is the approximation of the value of a linear operator L from $C_0^k[a,b]$ to a normed space W, where $C_0^k[a,b] = \{f:\ [a,b] \to R;\ f^{(k)}\ \textit{continuous}\ ;\ f^{(l)}(a) = 0,\ l = 0, 1, \cdots, k\}$. In particular, for integration $W = R$ and L is a linear functional, for function approximation $W = C_0^k[a,b]$ and L is the identity mapping I, and for derivative function approximation $W = C_0^{k-1}[a,b]$ and L is the derivative operator D. For a given input $f \in C_0^k[a,b]$, an algorithm is allowed to evaluate f at any point $x \in [a,b]$. Let $A_n(f) \in W$ be the approximation to $L(f)$ computed by the algorithm using values of f at n points $\{t_i\}_{i=1}^n$ where $a = t_0 < t_1 < t_2 < \cdots < t_n = b$. We assume that the partition $\{t_i\}_{i=0}^n$ of $[a,b]$ and the approximation A_n satisfy the following assumptions.

Assumption A There exist constants $\tilde{c}_1 > 0$ and $\tilde{c}_2 > 0$, such that

$$\tilde{c}_1 \le \frac{h_i}{h_{i-1}} \le \tilde{c}_2 \qquad (1)$$

where $h_i = t_i - t_{i-1}$, $i = 1, 2, \cdots, n$.

Assumption B The interval $[a,b]$ is divided into N panels $[T_0, T_1]$, $[T_1, T_2]$, ... , $[T_{N-1}, T_N]$, where $T_i = t_{il}$, $i = 0, 1, \cdots, N$, $N = n/l$, and l is a fixed positive integer that divides n. There exist constants $c_{Nj} \geq 0$, $j = 1, 2, \cdots, N$, bounded above by a constant independent of N, and a positive integer p, such that

$$||L(f) - A_n(f)||_W \leq \sum_{j=1}^{N} c_{Nj} H_j^p \sup_{T_{j-1} \leq t \leq T_j} |f^{(k)}(t)| \tag{2}$$

for any $f \in C_0^k[a,b]$. Here $H_j = T_j - T_{j-1}$, $j = 1, 2, \cdots, N$, and $||.||_W$ denotes the norm of W.

Assumption B is valid for various piecewise (composite) polynomial approximation methods, e.g., piecewise Lagrange interpolation, composite Newton-Cotes or Gauss rules, etc.

The *a posteriori* error criterion in Theorem 1 is a slight modification of the following heuristic divided difference test obtained by replacing the maximum of the kth derivative over $[T_{j-1}, T_j]$ in (2) with the maximum of the adjacent kth divided differences:

$$||L(f) - A_n(f)||_W \approx \sum_{j=1}^{N} c_{Nj} H_j^p \max_{\substack{1 \leq i \leq n \\ [t_{i-k}, t_i] \cap [T_{j-1}, T_j] \neq \phi}} | [t_{i-k}, t_{i-k+1}, \cdots, t_i] f | \tag{3}$$

for any $f \in C_0^k[a,b]$. Here $[t_{i-k}, t_{i-k+1}, \cdots, t_i] f$ is the kth divided difference of f at $t_{i-k}, t_{i-k+1}, \cdots, t_i$. The divided differences are defined recursively as

$$[t_{i-j}, t_{i-j+1}, \cdots, t_i] f = \frac{[t_{i-j+1}, t_{i-j+2}, \cdots, t_i] f - [t_{i-j}, t_{i-j+1}, \cdots, t_{i-1}] f}{t_i - t_{i-j}} \tag{4}$$

$i = 1, 2, \cdots, n$, $j \geq 1$; and $[t_i] f = f(t_i)$, for all i. We use the convention $t_{-i} = 2a - t_i$, and $f(t_{-i}) = 0$, $i > 0$, for divided differences near the interval endpoint a.

Let s_f be the natural spline interpolant of f at points $\{t_i\}_{i=1}^n$ in the Hilbert space $H_0^{k+1}[a,b] = \{g \in C_0^k[a,b] : g^{(k+1)} \in L_2[a,b]\}$. Namely, s_f is the (unique) element of $H_0^{k+1}[a,b]$ that satisfies the constraints $s_f(t_i) = f(t_i)$, $i = 1, 2, \cdots, n$, and

$$||s_f||_H = \inf_{\substack{g \in H_0^{k+1}[a,b] \\ g(t_i)=f(t_i) \\ i=1,2,\cdots,n}} ||g||_H$$

where $||.||_H = (<.,.>_H)^{1/2}$ is the norm of $H_0^{k+1}[a,b]$ and $<g,\, h>_H = \int_a^b g^{(k+1)}(t)h^{(k+1)}(t)\,dt$ is the inner product of $H_0^{k+1}[a,b]$. A reference on the natural splines is Prenter (1975). The relation between the natural spline interpolation and the best quadrature in the sense of Sard was studied in, among others, Schoenberg (1969), and Karlin (1969).

We have the following main theorem.

Theorem 1 There exists a constant $c > 0$ such that

$$||L(s_f) - A_n(f)||_W \leq c \sum_{j=1}^{N} c_{Nj}\, H_j^{p-1/2} \max_{\substack{1 \leq i \leq n \\ [t_{i-k}, t_i] \cap [T_{j-1}, T_j] \neq \phi}} |\, [t_{i-k},\, t_{i-k+1}, \cdots, t_i]\, f\,| \tag{5}$$

for any $f \in C_0^k[a,b]$.

In numerical approximation, often it is reassuring to know that one's computed solution is close to the solution of a different method. In fact, many automatic quadrature algorithms use as an *a posteriori* error criterion the local differences between the approximate solution and another local approximation obtained by a different quadrature. Our result is stronger. By Theorem 1, as an *a posteriori* error criterion the right-hand-side formula in (5) guarantees that the approximate solution is globally close to another approximation that has a minimal-norm property. Furthermore, this other solution need not even be computed explicitly, and the error criterion employed to achieve this is a sum of local error checks just as in many other algorithms in practice (see, e.g., Davis & Rabinowitz (1984)).

The following probabilistic result for the case of numerical integration is a corollary of Theorem 1. Its proof and more details of the probabilistic theory are in Gao (1990).

Corollary 1 Let $W = R$, and $||\alpha||_W = |\alpha|$, for any $\alpha \in R$, and let $L(f) = \int_a^b f(t)\,dt$, and $A(f) = Q_n(f) := \sum_{i=1}^{n} a_i f(t_i)$, for any $f \in C_0^k[a,b]$. Assume that the likelihood of an arbitrary

$f \in C_0^k[a,b]$ is distributed according to the Wiener measure on $C_0^k[a,b]$. Then there exist $b_{Nj} > 0$, $j = 1, 2, \cdots, N$, bounded above by a constant independent of N, such that,

$$\underset{\substack{g \in C_0^k[a,b] \\ g(x_i)=f(x_i) \\ i=1,2,\cdots,m}}{Average} \left|\int_a^b g(t)dt - Q_n(g)\right|^2 \le \sum_{j=1}^{N} b_{Nj}\, H_j^{2p+1}$$

$$+ \left(c \sum_{j=1}^{N} c_{Nj}\, H_j^{p-1/2} \max_{\substack{1 \le i \le n \\ [t_{i-k}, t_i] \cap [T_{j-1}, T_j] \ne \phi}} \left| [t_{i-k}, t_{i-k+1}, \cdots, t_i] f \right| \right)^2 \qquad (6)$$

for any $f \in C_0^k[a,b]$.

Also a corollary to Theorem 1, the next theorem concerns the near-optimality of the solution in the case of numerical integration. Again let $W = R$, and $||\alpha||_W = |\alpha|$, for any $\alpha \in R$, and let $L(f) = \int_a^b f(t)dt$, and $A_n(f) = Q_n(f) := \sum_{i=1}^{n} a_i f(t_i)$, for any $f \in C_0^k[a,b]$. For any constant $M > ||s_f||_H$, let $m(M;\{t_i\}_{i=1}^n) = \inf_{\{b_i\}} \sup_{\substack{g \in H_0^{k+1}[a,b] \\ g(t_i)=f(t_i) \\ i=1,2,\cdots,n \\ ||g||_H \le M}} \left|\int_a^b g(t)dt - \sum_{i=1}^{n} b_i f(t_i)\right|$, the minimal worst-case error on the set of integrands $\{g \in H_0^{k+1}[a,b]\colon g(t_i)=f(t_i),\ i = 1, 2, \cdots, n;\ ||g||_H \le M\}$ over all quadratures that use the same points of function evaluation $\{t_i\}_{i=1}^n$.

Theorem 2 For any given $(f(t_1), f(t_2), \cdots, f(t_n))^T \in R^n$,

$$\sup_{\substack{g \in H_0^{k+1}[a,b] \\ g(t_i)=f(t_i) \\ i=1,2,\cdots,n \\ ||g||_H \le M}} \left|\int_a^b g(t)dt - Q_n(f)\right| \le m(M;\{t_i\}_{i=1}^n) + c \sum_{j=1}^{N} c_{Nj}\, H_j^{p-1/2} \max_{\substack{1 \le i \le n \\ [t_{i-k}, t_i] \cap [T_{j-1}, T_j] \ne \phi}} \left| [t_{i-k}, t_{i-k+1}, \cdots, t_i] f \right| \qquad (7)$$

2. Proof of the theorems

Lemma 1 Under assumption A, there exists a constant $e > 0$ such that

$$\max_{\substack{1 \le i \le n \\ [t_{i-k-1}, t_i] \cap (T_{j-1}, T_j) \ne \phi}} \left| [t_{i-k-1}, t_{i-k}, \cdots, t_i] f \right| \le e\, H_j^{-1} \max_{\substack{1 \le i \le n \\ [t_{i-k}, t_i] \cap [T_{j-1}, T_j] \ne \phi}} \left| [t_{i-k}, t_{i-k+1}, \cdots, t_i] f \right| \qquad (8)$$

for any $f \in C_0^k[a,b]$.

Proof By the recursive definition of the divided differences (4), for any $q: [t_{q-k-1}, t_q] \cap (T_{j-1}, T_j) \neq \phi$,

$$| [t_{q-k-1}, t_{q-k}, \cdots, t_q] f | = \frac{| [t_{q-k}, t_{q-k+1}, \cdots, t_q] f - [t_{q-k-1}, t_{q-k}, \cdots, t_{q-1}] f |}{t_q - t_{q-k-1}}$$

$$\leq \frac{2 \max\limits_{\substack{1 \leq i \leq n \\ [t_{i-k-1}, t_i] \cap [T_{j-1}, T_j] \neq \phi}} |[t_{i-k}, t_{i-k+1}, \cdots, t_i] f |}{t_q - t_{q-k-1}}$$

$$\leq e H_j^{-1} \max_{\substack{1 \leq i \leq n \\ [t_{i-k-1}, t_i] \cap [T_{j-1}, T_j] \neq \phi}} | [t_{i-k}, t_{i-k+1}, \cdots, t_i] f | \tag{9}$$

where (9) follows by Assumption A. Q.E.D.

Lemma 2 There exists constants $d_1 > 0$, $d_2 > 0$, and $d_3 > 0$, such that for any $f \in C_0^k[a, b]$,

$$||L(s_f) - A_n(f)||_W \leq d_1 \sum_{i=1}^{N} c_{Nj} H_j^p \max_{\substack{1 \leq i \leq n \\ [t_{i-k}, t_i] \cap [T_{j-1}, T_j] \neq \phi}} | [t_{i-k}, t_{i-k+1}, \cdots, t_i] f |$$

$$+ d_2 \sum_{j=1}^{N} c_{Nj} H_j^{p+1/2} \left(\int_{\eta_j}^{\theta_j} (s_f^{(k+1)}(t))^2 dt \right)^{1/2} \tag{10}$$

for some η_j, θ_j, $j = 1, 2, \cdots, N$, where $\theta_j \in [T_{j-1}, T_j]$ and

$$|\eta_j - \theta_j| \leq d_3 H_j \tag{11}$$

Proof For every j: $1 \leq j \leq N$, let $\theta_j \in [T_{j-1}, T_j]$ be such that $s_f^{(k)}(\theta_j) = \sup\limits_{T_{j-1} \leq t \leq T_j} |s_f^{(k)}(t)|$, and choose any one $[t_{q-k}, t_{q-k+1}, \cdots, t_q] f$ such that $[t_{q-k}, t_q] \cap [T_{j-1}, T_j] \neq \phi$. By a well known fact of divided differences (see, e.g., Gao (1989)), there exists $\eta_j \in (t_{q-k}, t_q)$ such that $s_f(\eta_j) = k! \, [t_{q-k}, t_{q-k+1}, \cdots, t_q] f$. It follows from Assumption A that there exists a constant $d_3 > 0$ such that $|\eta_j - \theta_j| \leq d_3 H_j$. Thus, by Assumption B,

$$||L(s_j) - A_n(f)||_W \le \sum_{j=1}^{N} c_{Nj}\, H_j^p \sup_{T_{j-1}\le t\le T_j} |f^{(k)}(t)|$$

$$\le \sum_{j=1}^{N} c_{Nj}\, H_j^p \left(k!\, |\, [t_{q-k}, t_{q-k+1}, \cdots, t_q]\, f\,| + |\int_{\eta_j}^{\theta_j} s_j^{(k+1)}(t)\, dt|\right)$$

$$\le \sum_{j=1}^{N} c_{Nj}\, H_j^p\, k! \max_{\substack{1\le i\le n \\ [t_{i-k}, t_i]\cap[T_{j-1}, T_j]\ne\phi}} |\, [t_{i-k}, t_{i-k+1}, \cdots, t_i]\, f\,| + \sum_{j=1}^{N} c_{Nj}\, H_j^p |\eta_j - \theta_j|^{1/2} \left(\int_{\eta_j}^{\theta_j} (s_j^{(k+1)}(t))^2 dt\right)^{1/2}$$

$$\le k! \sum_{j=1}^{N} c_{Nj}\, H_j^p \max_{\substack{1\le i\le n \\ [t_{i-k}, t_i]\cap[T_{j-1}, T_j]\ne\phi}} |\, [t_{i-k}, t_{i-k+1}, \cdots, t_i]\, f\,| + d_3^{1/2} \sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2} \left(\int_{\eta_j}^{\theta_j} (s_j^{(k+1)}(t))^2 dt\right)^{1/2}$$

Q.E.D.

Lemma 3 There exists a constant $\bar{c} > 0$ such that

$$\sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2} \left(\int_{\eta_j}^{\theta_j} (s_j^{(k+1)}(t))^2 dt\right)^{1/2} \le \bar{c} \sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2} \max_{\substack{1\le i\le n \\ [t_{i-k-1}, t_i]\cap(T_{j-1}, T_j)\ne\phi}} |\, [t_{i-k-1}, t_{i-k}, \cdots, t_i]\, f\,| \quad (12)$$

for any $f \in C_0^k[a,b]$.

Proof The following is true of the natural splines (see, e.g., Gao (1989)): for any given $f \in C_0^k[a,b]$, there exist coefficients $b_i \in R^n$, $i = 1, 2, \cdots, n$, such that $s_j^{(k+1)}(t) = \sum_{i=1}^{n} b_i B_i(t)$, for any $t \in [a,b]$. Here $\{B_i(t)\}_{i=1}^{n}$ are the B-splines, i.e.,

$$B_i(t) = (-1)^{k+1} [t_{i-k-1}, t_{i-k}, \cdots, t_i]_x\, (t - x)_+^k$$

where the $(k+1)$st divided difference $[t_{i-k-1}, t_{i-k}, \cdots, t_i]_x$ operates on the variable x in $(t - x)_+^k$, $i = 1, 2, \cdots, n$, and

$$(t - x)_+^k = \begin{cases} 0, & t \le x \\ (t - x)^k, & t > x \end{cases}$$

$B_i(t)$ has the property that it vanishes outside $[t_{i-k-1}, t_i]$; also, let $N_i(t) = \Lambda_i^{1/2} B_i(t)$, where $\Lambda_i = t_{i-k-1} - t_i$, then

$$\int_{-\infty}^{\infty} (N_i(t))^2 dt \le 1, \qquad i = 1, 2, \cdots, n \quad (13)$$

(see, e.g., de Boor (1976)). Hence,

$$\sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2}\Big(\int_{\eta_j}^{\theta_j}(s_f^{(k+1)}(t))^2 dt\Big)^{1/2} = \sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2}\Big(\int_{\eta_j}^{\theta_j}\Big(\sum_{i=1}^{n} b_i B_i(t)\Big)^2 dt\Big)^{1/2}$$

$$= \sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2}\Big(\int_{\eta_j}^{\theta_j}\Big(\sum_{\substack{1\le i\le n\\ [t_{i-k-1},t_i]\bigcap(\eta_j,\theta_j)\ne\phi}} b_i B_i(t)\Big)^2 dt\Big)^{1/2}$$

$$\le \overline{c}_1\sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2}\Big(\sum_{\substack{1\le i\le n\\ [t_{i-k-1},t_i]\bigcap(\eta_j,\theta_j)\ne\phi}} \Lambda_i^{-1} b_i^2\Big)^{1/2} \tag{14}$$

for some constant $\overline{c}_1 > 0$, where (14) follows from (13) and (11), noting that by (11) the sum $\sum_{\substack{1\le i\le n\\ [t_{i-k-1},t_i]\bigcap(\eta_j,\theta_j)\ne\phi}}$ has only a constant number of terms. Here without loss of generality it is assumed that $\eta_j < \theta_j$. Furthermore,

$$\overline{c}_1\sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2}\Big(\sum_{\substack{1\le i\le n\\ [t_{i-k-1},t_i]\bigcap(\eta_j,\theta_j)\ne\phi}} \Lambda_i^{-1} b_i^2\Big)^{1/2} \le \overline{c}_1\Big(\sum_{j=1}^{N} H_j\Big)^{1/2}\Big(\sum_{j=1}^{N} c_{Nj}^2\, H_j^{2p}\Big(\sum_{\substack{1\le i\le n\\ [t_{i-k-1},t_i]\bigcap(\eta_j,\theta_j)\ne\phi}} \Lambda_i^{-1} b_i^2\Big)\Big)^{1/2}$$

$$\le \overline{c}_1 (b-a)^{1/2}\Big(\sum_{i=1}^{n} \Lambda_i^{-1} b_i^2 \sum_{\substack{1\le j\le N\\ (\eta_j,\theta_j)\bigcap[t_{i-k-1},t_i]\ne\phi}} c_{Nj}^2 H_j^{2p}\Big)^{1/2}$$

$$= \overline{c}_1 (b-a)^{1/2}\Big(\sum_{i=1}^{n} \Gamma_i\, \Lambda_i^{-1} b_i^2\Big)^{1/2} \tag{15}$$

where

$$\Gamma_i = \sum_{\substack{1\le j\le n\\ (\eta_j,\theta_j)\bigcap[t_{i-k-1},t_i]\ne\phi}} c_{Nj}^2\, H_j^{2p}, \qquad i = 1, 2, \cdots, n.$$

On the other hand,

$$[t_{i-k-1}, t_{i-k}, \cdots, t_i]\, f = \frac{1}{k!}\int_{-\infty}^{\infty} B_i(t)\, s_f^{(k+1)}(t)\, dt$$

(see, e.g., de Boor (1976))

$$= \frac{1}{k!}\int_{-\infty}^{\infty} B_i(t) \sum_{j=1}^{n} b_j B_j(t)\, dt$$

Let $G_B = (\tilde{b}_{ij})_{n\times n}$, where

$$\tilde{b}_{ij} = \int_{-\infty}^{\infty} B_i(t) B_j(t)\, dt, \qquad i, j = 1, 2, \cdots, n,$$

and $G_N = (\tilde{n}_{ij})_{n\times n}$, where

$$\tilde{n}_{ij} = \int_{-\infty}^{\infty} N_i(t) N_j(t)\, dt, \qquad i, j = 1, 2, \cdots, n,$$

and let

$$\Delta^k f = ([t_{-k}, t_{-k+1}, \cdots, t_1]\, f, [t_{-k+1}, t_{-k+2}, \cdots, t_2]\, f, \cdots, [t_{n-k+1}, t_{n-k}, \cdots, t_n]\, f)^T$$

and $b = (b_1, b_2, \cdots, b_n)^T$. Also denote by $Diag(\tilde{d}_i)$ a diagonal matrix whose diagonal entries are $\tilde{d}_1, \tilde{d}_2, \cdots, \tilde{d}_n$. Then,

$$\begin{aligned} k!\, \Delta^k f &= G_B\, b \\ &= Diag(\Lambda_i^{-1/2})\, G_N\, Diag(\Lambda_i^{-1/2})\, b \\ &= Diag(\Gamma_i^{-1/2}\Lambda_i^{-1/2})\, Diag(\Gamma_i^{1/2})\, G_N\, Diag(\Gamma_i^{-1/2})\, Diag(\Gamma_i^{1/2}\Lambda_i^{-1/2})\, b \end{aligned}$$

Therefore,

$$Diag(\Gamma_i^{1/2}\Lambda_i^{-1/2})\, b = Diag(\Gamma_i^{1/2})\, G_N^{-1}\, Diag(\Gamma_i^{-1/2})\, Diag(\Gamma_i^{1/2}\Lambda_i^{1/2})\, k!\, \Delta^k f$$

By (14) and (15),

$$\begin{aligned} \sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2} \Big(\int_{\eta_j}^{\theta_j} (s_j^{(k+1)}(t))^2 dt\Big)^{1/2} &\le \bar{c}_1 (b-a)^{1/2}\, \|Diag(\Gamma_i^{1/2}\Lambda_i^{-1/2})\, b\|_2 \\ &\le \bar{c}_1 (b-a)^{1/2} k!\, \|Diag(\Gamma_i^{1/2})\, G_N^{-1}\, Diag(\Gamma_i^{-1/2})\|_2\, \|Diag(\Gamma_i^{1/2}\Lambda_i^{1/2})\, \Delta^k f\|_2 \\ &= \bar{c}_1 (b-a)^{1/2}\, \|G_N^{-1}\|_2\, \|Diag(\Gamma_i^{1/2}\Lambda_i^{1/2})\, \Delta^k f\|_2 \qquad (16) \end{aligned}$$

where (16) holds because a similarity transformation does not alter the 2-norm of a symmetric matrix. By de Boor (1976), there exists a constant $\bar{c}_2 > 0$ such that

$$\|G_N^{-1}\|_2 \le \bar{c}_2$$

Thus,

$$\sum_{j=1}^{N} c_{Nj}\, H_j^{p+1/2} \Big(\int_{\eta_j}^{\theta_j} (s_j^{(k+1)}(t))^2 dt\Big)^{1/2} \le \bar{c}_1 (b-a)^{1/2} \bar{c}_2\, k!\, \|Diag(\Gamma_i^{1/2}\Lambda_i^{1/2})\, \Delta^k f\|_2$$

$$= \overline{c}_1 (b-a)^{1/2} \overline{c}_2\, k!\, (\sum_{i=1}^{n} (t_{i-k-1} - t_i) ([t_{i-k-1}, t_{i-k}, \cdots, t_i] f)^2 (\sum_{\substack{1 \le j \le N \\ (\eta_j, \theta_j) \cap [t_{i-k-1}, t_i] \neq \phi}} c_{Nj}^2 H_j^{2p}))^{1/2}$$

$$= \overline{c}_1 (b-a)^{1/2} \overline{c}_2\, k!\, (\sum_{j=1}^{N} c_{Nj}^2 H_j^{2p} (\sum_{\substack{1 \le i \le n \\ [t_{i-k-1}, t_i] \cap (\eta_j, \theta_j) \neq \phi}} (t_{i-k-1} - t_i) ([t_{i-k-1}, t_{i-k}, \cdots, t_i] f)^2))^{1/2}$$

$$\le \overline{c}_1 (b-a)^{1/2} \overline{c}_2\, k! \sum_{j=1}^{N} c_{Nj} H_j^{p} (\sum_{\substack{1 \le i \le n \\ [t_{i-k-1}, t_i] \cap (\eta_j, \theta_j) \neq \phi}} (t_{i-k-1} - t_i)^{1/2} \, | [t_{i-k-1}, t_{i-k}, \cdots, t_i] f |)$$

$$\le \overline{c} \sum_{j=1}^{N} c_{Nj} H_j^{p+1/2} \max_{\substack{1 \le i \le n \\ [t_{i-k-1}, t_i] \cap (T_{j-1}, T_j) \neq \phi}} | [t_{i-k-1}, t_{i-k}, \cdots, t_i] f | \qquad (17)$$

where (17) is obtained using (11) and Assumption A. Q.E.D.

Proof of Theorem 1 Apply Lemmas 2, 3 and 1 in that order. Q.E.D.

Proof of Theorem 2 Given $(f(t_1), f(t_2), \cdots, f(t_n))^T \in R^n$, for any $g \in H_0^{k+1}[a,b]$, $g(t_i) = f(t_i)$, $i = 1, 2, \cdots, n$,

$$|\int_a^b g(t)\,dt - Q_n(f)| \le |\int_a^b g(t)\,dt - \int_a^b s_f(t)\,dt| + |\int_a^b s_f(t)\,dt - Q_n(f)|$$

$$\le |\int_a^b g(t)\,dt - \int_a^b s_f(t)\,dt| + c \sum_{j=1}^{N} c_{Nj} H_j^{p-1/2} \max_{\substack{1 \le i \le n \\ [t_{i-k}, t_i] \cap [T_{j-1}, T_j] \neq \phi}} | [t_{i-k}, t_{i-k+1}, \cdots, t_i] f |$$

by Theorem 1. Thus it suffices to show that

$$m(M; \{t_i\}_{i=1}^n) = \sup_{\substack{g \in H_0^{k+1}[a,b] \\ g(t_i) = f(t_i) \\ i=1,2,\cdots,n \\ ||g||_H \le M}} |\int_a^b g(t)\,dt - \int_a^b s_f(t)\,dt|$$

i.e., the spline interpolation solution minimizes worst-case error on the set of integrands $\{g \in H_0^{k+1}[a,b]: g(t_i) = f(t_i),\ i = 1, 2, \cdots, n;\ ||g||_H \le M\}$ among all quadratures that use the same points of function evaluation $\{t_i\}_{i=1}^n$. Indeed,

$$\sup_{\substack{g \in H_0^{k+1}[a,b] \\ g(t_i) = f(t_i) \\ i=1,2,\cdots,n \\ ||g||_H \le M}} |\int_a^b g(t)\,dt - \sum_{i=1}^{n} b_i f(t_i)| = \sup_{\substack{h \in H_0^{k+1}[a,b] \\ h(t_i) = 0 \\ i=1,2,\cdots,n \\ ||h+s_f||_H \le M}} |\int_a^b h(t)\,dt + \int_a^b s_f(t)\,dt - \sum_{i=1}^{n} b_i f(t_i)|$$

$$= \sup_{\substack{h \in H_0^{k+1}[a,b] \\ h(t_i)=0 \\ i=1,2,\cdots,n \\ \|h\|_H \le (M^2 - \|s_f\|_H^2)^{1/2}}} \left| \int_a^b h(t)\,dt + \int_a^b s_f(t)\,dt - \sum_{i=1}^n b_i f(t_i) \right| \qquad (18)$$

where (18) holds because of an elementary fact of the natural splines that $<s_f, h>_H = 0$, for any $h \in H_0^{k+1}[a,b]$, $h(t_i) = 0$, $i = 1, 2, \cdots, n$ (see, e.g., Prenter (1975)), and therefore $\|h+s_f\|_H^2 = \|h\|_H^2 + \|s_f\|_H^2$.

Since the set $\{h \in H_0^{k+1}[a,b]\colon h(t_i)=0,\ i = 1, 2, \cdots, n;\ \|h\|_H \le (M^2 - \|s_f\|_H^2)^{1/2}\}$ is convex and balanced, the right hand side of (18) is minimized by choosing $\{b_i\}_{i=1}^n$ such that

$$\sum_{i=1}^n b_i f(t_i) - \int_a^b s_f(t)\,dt = 0.$$

Arguments of this type can be found in, e.g., Micchelli & Rivlin (1985), and Traub & Wozniakowski (1980). Q.E.D.

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