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Stable integration rules with scattered integration points

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Abstract

A general method for near-best approximations to functionals on $\mathbb{R}^d$, using scattered-data information, is applied for producing stable multidimensional integration rules. The rules are constructed to be exact for polynomials of degree $\leqslant m$ and, for a quasi-uniform distribution of the integration points, it is shown that the approximation order is $O(h^{m+1})$ where h is an average distance between the data points. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

Given function values at scattered data points in a domain we are sometimes asked to evaluate the integral of the function over the domain. The common practice in such a case is to approximate the function by some interpolation procedure and to integrate the interpolant. We suggest a direct approach to the integration problem, and our approach is based upon the following general method for approximation:

Let $f \in F$ where F is a normed function space on $\mathbb{R}^d$, and let $\{L_i(f)\}_{i=1}^N$ be a data set, where $\{L_i\}_{i=1}^N$ are bounded linear functionals on F. In most problems in approximation we are looking for an approximation to $L(f)$, where L is another bounded linear functional on F, in terms of the given data $\{L_i(f)\}_{i=1}^N$. Usually we choose a set of basis functions, $\{\phi_k\} \subset F$, e.g., polynomials, splines, or radial basis functions. Then we find an approximation $\hat{f}$ to f from span$\{\phi_k\}$, and approximate $L(f)$ by $L(\hat{f})$. If the approximation process is linear, the final approximation can be expressed as

$$\hat{L}(f) \equiv L(\hat{f}) = \sum_{i=1}^{N} a_i L_i(f). \tag{1.1}$$

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In analyzing the approximation error, or the approximation order, we are frequently using the fact that the approximation procedure is exact for a finite set of fundamental functions $P \equiv \mathrm{span}\{p_j\}_{j=1}^J \subset F$. Usually, we choose P to be Π_m, the space of polynomials of total degree $\leqslant m$.

$$\hat{L}(p) = \sum_{i=1}^{N} a_i L_i(p) = p, \ \ p \in P. \tag{1.2}$$

In case the basis functions $\{\phi_k\} \subset F$ are locally supported (e.g., B-splines) and $P = \Pi_m$, and under some proper assumptions on the distribution of the data points, it can be shown that the resulting approximation error is $O(h^{m+1})$, where h is an average distance between the data points. Another way of analyzing the approximation error follows directly from the representation (1.1).

Let $\Omega_0 \subset \mathbb{R}^d$ be the support of the functional L, i.e. $L(g) = 0$ for all g vanishing on Ω_0, and let Ω_N denote the support of $\sum_{i=1}^N a_i L_i$. Also let p be the best approximation to f from the set P on $\Omega \equiv \Omega_0 \cup \Omega_N$,

$$E_{\Omega,P}(f) \equiv \|f - p\|_\Omega = \inf_{q \in P} \|f - q\|_\Omega, \tag{1.3}$$

where $\|\cdot\|_\Omega$ is the natural restriction to Ω of the norm on F. Using (1.2) it follows that

$$\begin{aligned} |L(f) - \hat{L}(f)| &\leqslant |L(f) - L(p)| + |L(p) - \hat{L}(f)| \\ &\leqslant \|L\| \|f - p\|_\Omega + \left| \sum_{i=1}^{N} a_i L_i(f - p) \right| \\ &\leqslant \|L\| \|f - p\|_\Omega + \sum_{i=1}^{N} |a_i| \|L_i\| \|f - p\|_\Omega \\ &= \left(\|L\| + \sum_{i=1}^{N} |a_i| \|L_i\| \right) E_{\Omega,P}(f). \end{aligned} \tag{1.4}$$

Thus, a bound on the error, in the approximation (1.1) is given in terms of the norms of L and the L_i's, the coefficients $\{a_i\}_{i=1}^N$, and of $E_{\Omega,P}(f)$, the error of best approximation to f on Ω from P. Similarly, let $\tilde{p}$ be the best approximation to f on Ω from all $q \in P$ such that $L(q) = L(f)$, and let

$$E^L_{\Omega,P}(f) \equiv \|f - \tilde{p}\|_\Omega = \inf_{q \in P, L(q) = L(f)} \|f - q\|_\Omega. \tag{1.5}$$

Then it follows that

$$|L(f) - \hat{L}(f)| \leqslant \sum_{i=1}^{N} |a_i| \|L_i\| E^L_{\Omega,P}(f). \tag{1.6}$$

Let us assume that the data set $\{L_i(f)\}_{i=1}^N$ is finite and $J \leqslant N$. In [6] we use the Backus–Gilbert approach [1–4], to find the coefficients vector $\bar{a} = \{a_1, \ldots, a_N\}$ for the approximation $\hat{L}(f) = \sum_{i=1}^N a_i L_i(f)$ by minimizing the quadratic form

$$Q = \sum_{i=1}^{N} w(L_i, L) a_i^2, \tag{1.7}$$

subject to the linear constraints

$$\sum_{i=1}^{N} a_i L_i(p_j) = L(p_j), \quad j = 1,\ldots,J. \tag{1.8}$$

In (1.7) $\{w(L_i,L)\}$ are non-negative weights, $w(L_i,L)$ represents a separation measure between the functionals L_i and L, $w(L_i,L) > 0$ if $L_i \neq L$.

Assume $L \neq L_k$, $k = 1,\ldots,N$, and $\mathrm{Rank}(E) = J$ where $E_{i,j} = L_i(p_j)$ for $1 \leqslant i \leqslant N$, $1 \leqslant j \leqslant J$. It is shown in [6] that the approximation defined by the constraint minimization problem (1.7), (1.8) is $\hat{L}(f) = \sum_{i=1}^{N} a_i L_i(f)$ with

$$\bar{a} = D^{-1}E(E^t D^{-1} E)^{-1}\bar{c}, \tag{1.9}$$

where $D = 2\mathrm{Diag}\{w(L_1,L),\ldots,w(L_N,L)\}$ and $\bar{c} = (L(p_1),\ldots,L(p_J))^{\mathrm{t}}$. A typical example is the interpolation problem, where $\{L_i\}$ and L are the point evaluation functionals, $L_i(f) = f(x_i)$, $1 \leqslant i \leqslant N$, and $L(f) = f(x)$. In this case, we take $w(L_i,L) = \eta(\|x - x_i\|)$, where $\eta(t)$ is fast decreasing as $t \to \infty$, and it is important to note that $a_i = a_i(x)$, $1 \leqslant i \leqslant N$. Namely, the coefficients in the approximating functional $\hat{L}$ vary with the point x.

The resulting approximant is closely related to the moving least-squares method of McLain [8,9], which is further discussed by Lancaster and Salkauskas [7]. In [6] we demonstrate and analyze the method for univariate interpolation, smoothing and derivative approximation, and for scattered-data interpolation and derivative approximation in $\mathbb{R}^d$, $d = 2,3$. In the present work we suggest to use the method for deriving numerical integration rules based upon scattered-data information.

2. Integration formulas with scattered nodes

In this work we consider the approximation of

$$I(f,\Omega) = \int_{\Omega} w(x) f(x)\,\mathrm{d}x, \tag{2.1}$$

where Ω is a domain in $\mathbb{R}^d$, $w(x) \geqslant 0$ on Ω, and f is a smooth enough function. We assume that values of f are given on a set $X = \{x_i\}_{i=1}^{N} \subset \Omega$ and we look for an integration formula of the form

$$I_N(f,\Omega) = \sum_{i=1}^{N} A_i f(x_i). \tag{2.2}$$

Following [10] and [5], our goal is to achieve a formula which is stable, i.e., $\sum_i^N |A_i|$ is as small as possible, and for which we can prove an approximation order result. We restrict the discussion to sets of nodes as defined below.

Definition (*Sets h–ρ–δ, of mesh size h, density* $\leqslant \rho$, *and separation* $\geqslant h\delta$). Let Ω be a domain in $\mathbb{R}^d$, and consider sets of data points in Ω. We say that the set $X = \{x_i\}_{i=1}^{N}$ is a set h–ρ–δ if

1. h is the minimal number such that

$$\Omega \subset \bigcup_{i=1}^{N} B(x_i, h/2), \tag{2.3}$$

where $B(x,r)$ is the closed ball of radius r with center x.

2.
$$\#\{X \cap B(y, qh)\} \leqslant \rho q^d, \quad q \geqslant 1, \;\; y \in \Omega. \tag{2.4}$$

Here, $\#\{Y\}$ denotes the number of elements of a given set Y.

3. $\exists \delta > 0$ such that
$$\|x_i - x_j\| \geqslant h\delta, \quad 1 \leqslant i < j \leqslant N. \tag{2.5}$$

Let f be a function in $C^{m+1}(\Omega)$. Then, for sets h–ρ–δ of nodes, with fixed ρ and δ, we would like to get
$$|I(f,\Omega) - I_N(f,\Omega)| \leqslant C \cdot h^{m+1}, \tag{2.6}$$
as $h \to 0$.

Let us suppose that we know how to evaluate $I(p,\Omega)$ for $p \in \Pi_m$. Then, the obvious strategy for defining a good stable integration formula would be to find the weights $\{A_i\}$ in (2.2) such that
$$I_N(p,\Omega) = I(p,\Omega), \quad p \in \Pi_m, \tag{2.7}$$
and $\sum_{i=1}^N |A_i|$ is minimal. This problem is not well posed, and it usually has infinitely many solutions. It is not clear how to extract an integration rule which satisfies an approximation order result like (2.6). In the following, we suggest a composite rule strategy for building the integration formula (2.2). We decompose the domain Ω into subdomains of diameter $\mathrm{O}(h)$, $\Omega = \bigcup_{k=1}^K E_k$, $E_k \cap E_j = \emptyset$ for $k \neq j$. For each E_k we then construct an integration formula
$$I_N^m(f, E_k) = \sum_{i=1}^N A_i^{(k)} f(x_i) \approx I(f, E_k) \tag{2.8}$$
which is as local and as stable as possible. Then we aggregate all the local formulae into a global integration rule (2.2) over Ω with
$$A_i = \sum_{k=1}^K A_i^{(k)} \tag{2.9}$$
and we denote this rule by $I_N^m(f,\Omega)$. Note that the rule also depends upon the specific decomposition of Ω into subdomains. Following the general idea presented in the introduction we propose the following procedure for defining an integration formula of order m on a subdomain $E \subset \Omega$.

Let us assume that the integrals $I(p,E)$, for $p \in \Pi_m$, are easily computable, and let x^* be some center of E. We define an approximation $I_N^m(f,E) = \sum_i^N a_i f(x_i) \approx I(f,E)$ so that the rule is exact for Π_m, i.e.,
$$I_N^m(p,E) = I(p,E), \quad \forall p \in \Pi_m. \tag{2.10}$$
Furthermore, for the localization of the rule and for controlling the magnitudes of the weights we require that the $\{a_i\}$ minimize the quadratic form
$$Q = \sum_{i=1}^N \eta(\|x^* - x_i\|) a_i^2, \tag{2.11}$$

with a fast increasing, finitely supported, weight function

$$\eta(r) = \exp(r^2/h^2)\chi_s(r/h), \tag{2.12}$$

where χ_s is the characteristic function of the open ball of a radius s around $x = 0$, and s is some fixed number so that $E \subset B(x^*, sh)$.

In the framework of the general procedure presented in the Introduction, $L(f) = I(f, E)$ and $L_i(f) = f(x_i)$, $i = 1, \ldots, N$. Consequently, the solution of the constraint minimization problem (2.10) and (2.11) is given by (1.9), namely $\bar{a} = D^{-1}E(E^tD^{-1}E)^{-1}\bar{c}$ with

$$D = 2\mathrm{Diag}\{\eta(\|x^* - x_1\|), \ldots, \eta(\|x^* - x_N\|)\},$$

$$E_{i,j} = p_j(x_i), \quad 1 \leqslant i \leqslant N, \ 1 \leqslant j \leqslant J$$

and $\bar{c} = (I(p_1, E), \ldots, I(p_J, E))^t$. Here $J = \binom{d+m}{m}$ is the dimension of Π_m and the computation of the coefficients vector $\bar{a}$ involves the solution of a full linear system of order J.

In the following, we present an approximation order theorem for the resulting aggregated approximation to $I(f, \Omega)$, defined by (2.2) and (2.9) with weights $\{A_i^{(k)}\}$ defined as the coefficients $\{a_i\}$ obtained by the above process applied for $E = E_k$.

Theorem. *Let f be a function in $C^{m+1}(\Omega)$, and consider sets $h - \rho - \delta$ of data points with fixed ρ and δ. Then, there exists $h^* > 0$ such that the approximation $I_N^m(f, \Omega)$ defined by* (2.2) *and* (2.9), *with η given by* (2.12), *satisfies*

$$|I(f, \Omega) - I_N^m(f, \Omega)| \leqslant Ch^{m+1}, \tag{2.13}$$

for $0 < h \leqslant h^*$.

Proof. For a fixed h we decompose the domain Ω into subdomains of diameter $O(h)$, such that $\Omega = \bigcup_{k=1}^K E_k$, $E_k \cap E_j = \emptyset$ for $k \neq j$. As in [6] it can be shown that, for a sufficiently small h, there exists a fixed $s > 0$ (for the definition of η in (2.12)) such that the approximation on each subdomain $\{E_k\}$ satisfies

$$|I(f, E_k) - I_N^m(f, E_k)| \leqslant C_1 h^{m+1} \times \mathrm{Volume}(E_k) \leqslant C_2 h^{m+1+d}, \tag{2.14}$$

where C_1 and C_2 are constants independent of k and h. Summing up all the approximations $I_N^m(f, E_k)$, noting that there are $O(h^{-d})$ subdomains, the result (2.13) follows. □

3. Numerical demonstration — Scattered data integration rules in $\mathbb{R}^2$ and $\mathbb{R}^3$

In this section we present some results on the application of the suggested method for deriving integration formulae. We consider scattered nodes in domains in $\mathbb{R}^2$ and $\mathbb{R}^3$, and we try to show that the method gives good stable integration rules. We examined integration rules over $\Omega = [0, 1]^d$ based upon data points scattered in $[0, 1]^d$, for $d = 2, 3$, and obtained very good approximations for many test functions. The weight function η used in our experiments is

$$\eta(r) = \exp(r^2/h^2). \tag{3.1}$$

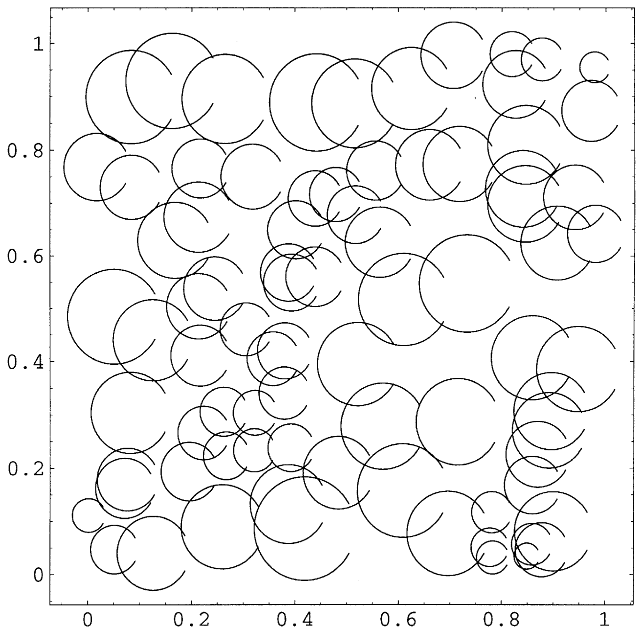

Fig. 1. The weights for the integration rule $I^3_{81}(f,\Omega)$.

In one of the experiments we applied the method for a set of 81 data points randomly chosen in $[0,1]^2$, with a corresponding $h=0.25$ in (3.1). In Fig. 1 we display the weights of the resulting integration rule (2.2) which is obtained as described in Section 2, with the exactness class Π_3 ($J=10$). We used the decomposition of $[0,1]^2$ into squares of size 0.25×0.25 and we denote this approximation by $I^3_{81}(f,\Omega)$. Each intergation point is represented by a circle of area equals the absolute value of the corresponding weight. The circles are open to the right if the weights are positive, and to the left if negative. We observe that the weights are all positive, and that there are larger weights where there are fewer data points. The application of the integration rule to the function $f(x,y)=\mathrm{e}^{x-y}$ yields a relative error ~ 0.000065, while for the function $f(x,y)=\mathrm{e}^{5(x-y)}$ the relative error is ~ 0.0317, which is consistent with an approximation order 4.

Similar properties were observed in the 3-D case. We applied the method of exactness class Π_2 in $\mathbb{R}^3$ ($J=10$) for a set of 729 integration points randomly chosen in $[0,1]^3$, with $h=0.25$ in (3.1). Here the subdomains are chosen to be boxes of size $0.25\times 0.25\times 0.25$. Here we choose to display the weights of the integration rule for the subdomain $E=[0.75,1]^3$. The weights are depicted in Fig. 2, where each integration point is represented by a box of size proportional to the value of the corresponding weight in the rule for $I^2_{729}(f,E)$. The boxes are open above if the corresponding weights are positive, and below if negative. We observe that the significant weights are all positive, and that they are all in a small neighborhood of the subdomain E. Here also all the weights of the integration rule $I^2_{729}(f,[0,1]^3)$ turn to be positive. We remark that this is not always true. However, the number and the magnitudes of the negative weights are always very small. The application of the integration rule to the function $f(x,y)=\mathrm{e}^{x-y+z}$ yields a relative error ~ 0.000165, while for the

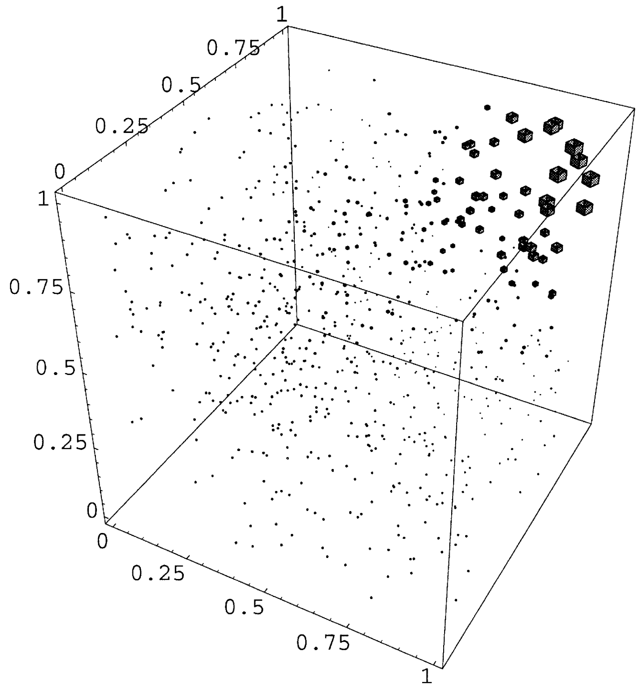

Fig. 2. The weights for the integration rule $I^2_{729}(f, [0.75, 1]^3)$.

function $f(x, y) = e^{5(x-y+z)}$ the relative error is ~ 0.0386, which is consistent with an approximation order 3.

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