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HERMITE–HADAMARD–TYPE INEQUALITIES IN THE APPROXIMATE INTEGRATION

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Abstract. We give a slight extension of the Hermite–Hadamard inequality on simplices and we use it to establish error bounds of the operators connected with the approximate integration.

1. Introduction

In the numerical analysis there are many classical quadrature rules. For each of them the error terms are well known. In the series of recent papers [4, 5, 6] the author established error bounds of quadrature operators under regularity assumptions weaker from the classical ones. The method was based on the use of Hermite–Hadamard–type inequalities for convex functions of higher order.

In this paper we develop an analogous idea for convex functions of several variables defined on simplices in $\mathbb{R}^n$. It is possible because the generalizations of the Hermite–Hadamard inequality are known for multiple integrals, e.g. by Choquet theory. Recently Bessenyei proved in [1] such an inequality on simplices using an elementary approach. We slightly extend this result and we use this extension to give error bounds of operators connected with the approximate computation of multiple integrals (i.e. the cubatures).

Let $p_0,\dots,p_n \in \mathbb{R}^n$ be affine independent and let S be a simplex with vertices $p_0,\dots,p_n$. Denote by $\overline{p}$ its barycenter, i.e.

$$\overline{p} := \frac{1}{n+1}\sum_{i=0}^{n} p_i$$

and by $\operatorname{vol}(S)$ its volume.

In our proofs we use some results contained in [1]. One of them is the following

LEMMA 1. *If $A:\mathbb{R}^n \to \mathbb{R}$ is an affine function then*

$$A(\overline{p}) = \frac{1}{\operatorname{vol}(S)}\int_S A(x)dx = \frac{1}{n+1}\sum_{i=0}^{n} A(p_i).$$

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The properties of convex functions needed in this paper can be found in many textbooks and monographs, for instance in [2] (cf. also [1]).

Recall that a linear functional $\mathscr{T}$ defined on a linear space X of (not necessarily all) functions mapping some nonempty set into $\mathbb{R}$ is called *positive* if

$$f \leqslant g \implies \mathscr{T}(f) \leqslant \mathscr{T}(g)$$

for any $f, g \in X$.

2. Hermite–Hadamard–type inequalities

We start with a slight generalization of the Hermite–Hadamard inequality.

THEOREM 2. *Let $\mathscr{T}$ be positive linear functional defined (at least) on a linear subspace of all functions mapping S into $\mathbb{R}$ generated by a cone of convex functions. Assume that*

$$\mathscr{T}(A) = \frac{1}{\operatorname{vol}(S)} \int_S A(x)dx$$

for any affine function $A : S \to \mathbb{R}$. Then the inequality

$$f(\overline{p}) \leqslant \mathscr{T}(f) \leqslant \frac{1}{n+1} \sum_{i=0}^{n} f(p_i)$$

holds for any convex function $f : S \to \mathbb{R}$.

Proof. By convexity the subdifferential $\partial f(\overline{p})$ is non–empty, whence there exists an affine function $A : S \to \mathbb{R}$ supporting f at the point $\overline{p}$ (i.e. $A(\overline{p}) = f(\overline{p})$ and $A \leqslant f$ on S). Using Lemma 1 and the properties of $\mathscr{T}$ we get

$$f(\overline{p}) = A(\overline{p}) = \frac{1}{\operatorname{vol}(S)} \int_S A(x)dx = \mathscr{T}(A) \leqslant \mathscr{T}(f).$$

Since $p_0, \ldots, p_n$ are affine independent, there exists (exactly one) affine function $B : S \to \mathbb{R}$ such that $B(p_i) = f(p_i)$, $i = 0, \ldots, n$. A simplex S is the convex hull of the set $\{p_0, \ldots, p_n\}$. Then by convexity $f \leqslant B$ on S. Using once again Lemma 1 and the properties of $\mathscr{T}$ we arrive at

$$\mathscr{T}(f) \leqslant \mathscr{T}(B) = \frac{1}{\operatorname{vol}(S)} \int_S B(x)dx = \frac{1}{n+1} \sum_{i=0}^{n} B(p_i) = \frac{1}{n+1} \sum_{i=0}^{n} f(p_i).$$

$\square$

As an immediate consequence we obtain the Hermite–Hadamard inequality.

COROLLARY 3. *If $f : S \to \mathbb{R}$ is convex then*

$$f(\overline{p}) \leqslant \frac{1}{\operatorname{vol}(S)} \int_S f(x)dx \leqslant \frac{1}{n+1} \sum_{i=0}^{n} f(p_i).$$

Another important consequence of Theorem 2 concerns the operators of the form of a convex combination of the values of f at some appropriately chosen points of S.

COROLLARY 4. *Let $m \in \mathbb{N}$, $\lambda_1, \ldots, \lambda_m \geqslant 0$ with $\sum_{i=1}^{m} \lambda_i = 1$ and $\xi_1, \ldots, \xi_m \in S$ with $\sum_{i=1}^{m} \lambda_i \xi_i = \overline{p}$. If a function $f : S \to \mathbb{R}$ is convex then*

$$f(\overline{p}) \leqslant \sum_{i=1}^{m} \lambda_i f(\xi_i) \leqslant \frac{1}{n+1} \sum_{i=0}^{n} f(p_i).$$

Proof. Clearly

$$\mathscr{T}(f) := \sum_{i=1}^{m} \lambda_i f(\xi_i)$$

is a positive linear functional. Let $A : S \to \mathbb{R}$ be an affine function. Then by Lemma 1

$$\mathscr{T}(A) = \sum_{i=1}^{m} \lambda_i A(\xi_i) = A\Big(\sum_{i=1}^{m} \lambda_i \xi_i\Big) = A(\overline{p}) = \frac{1}{\operatorname{vol}(S)} \int_S A(x)dx$$

and all the assumptions of Theorem 2 are fulfilled. □

This result is useful in the approximate computation of multiple integrals over S. Together with further results of this paper it allows us to give error bounds of the cubatures of the form of a conical combination of the values of an integrand at some points of S. These error bounds depend on the second order differential of the involved functions.

To conclude this section notice that in Theorem 2 not a form of an operator $\mathscr{T}$ is essential but three its properties are important: $\mathscr{T}$ is linear, positive and it coincides with the integral mean value in the class of affine functions.

3. A norm of a second order differential

Let $\varphi : \mathbb{R}^n \to \mathbb{R}$ be a quadratic form, i.e.

$$\varphi(x) = \sum_{i,j=1}^{n} a_{ij} x_i x_j$$

for $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$. Let

$$\|\varphi\| := \sup\big\{\big|\varphi(x)\big| : \|x\| = 1\big\}.$$

This is well defined norm on a linear space of all quadratic forms of n variables with the following properties:

$$\|\varphi\| \leqslant \sum_{i,j=1}^{n} |a_{ij}|,$$

$$\big|\varphi(x)\big| \leqslant \|\varphi\| \cdot \|x\|^2, \quad x \in \mathbb{R}^n.$$

The details may be easily checked (cf. e.g. [3]).

Now let $f \in \mathscr{C}^2(S)$. Then the partial derivatives of the second order are bounded, say, there exists a constant $M > 0$ such that

$$\left|\frac{\partial^2 f}{\partial x_i \partial x_j}(u)\right| \leqslant \frac{M}{n^2}$$

for any $u \in S$, $i,j = 1,\dots,n$. Then for any $u \in S$

$$d^2 f(u)(v,v) = \sum_{i,j=1}^{n} \frac{\partial^2 f}{\partial x_i \partial x_j}(u) v_i v_j,$$

whence

$$\left\|d^2 f(u)\right\| \leqslant \sum_{i,j=1}^{n} \left|\frac{\partial^2 f}{\partial x_i \partial x_j}(u)\right| \leqslant M.$$

This allows us to define

$$\|d^2 f\|_\infty := \sup_{u \in S} \left\|d^2 f(u)\right\|.$$

Obviously

$$\left\|d^2(f+g)\right\|_\infty \leqslant \|d^2 f\|_\infty + \|d^2 g\|_\infty, \tag{1}$$

$$\left\|d^2(\alpha f)\right\|_\infty = |\alpha| \cdot \|d^2 f\|_\infty, \tag{2}$$

$$\left|d^2 f(u)(v,v)\right| \leqslant \left\|d^2 f(u)\right\| \cdot \|v\|^2 \leqslant \|d^2 f\|_\infty \|v\|^2 \tag{3}$$

for any $f, g \in \mathscr{C}^2(S)$, $\alpha \in \mathbb{R}$, $u \in S$ and $v \in \mathbb{R}^n$.

LEMMA 5. *If $f \in \mathscr{C}^2(S)$ and $g(x) = \frac{\|d^2 f\|_\infty}{2}\|x\|^2$ then the functions $g+f$ and $g-f$ are convex. Moreover,*

$$\left\|d^2(g+f)\right\|_\infty \leqslant 2\|d^2 f\|_\infty \quad \textit{and} \quad \left\|d^2(g-f)\right\|_\infty \leqslant 2\|d^2 f\|_\infty.$$

Proof. It is easy to compute $d^2 g(u)(v,v) = \|d^2 f\|_\infty \|v\|^2$. Then by (3)

$$\left|d^2 f(u)(v,v)\right| \leqslant \|d^2 f\|_\infty \|v\|^2 = d^2 g(u)(v,v).$$

Hence, for any $u \in S$, $v \in \mathbb{R}^n$,

$$d^2(g+f)(u)(v,v) \geqslant 0 \quad \text{and} \quad d^2(g-f)(u)(v,v) \geqslant 0,$$

which means that for any $u \in S$, $d^2(g+f)(u)$ and $d^2(g-f)(u)$ are positive semi–definite. Then $g+f$ and $g-f$ are convex.

If $\|v\| = 1$ then $d^2g(u)(v,v) = \|d^2f\|_\infty$ for any $u \in S$, which implies $\|d^2g(u)\| = \|d^2f\|_\infty$, $u \in S$. Then $\|d^2g\|_\infty = \|d^2f\|_\infty$ and by (1), (2) we obtain the second assertion of the Lemma. □

4. Applications to the approximate integration

LEMMA 6. *If $f \in \mathscr{C}^2(S)$ then*

$$\left|\int_S f(x)dx - \operatorname{vol}(S) f(\overline{p})\right| \leqslant \frac{1}{2}\|d^2f\|_\infty \int_S \|x-\overline{p}\|^2 dx.$$

Proof. Write Taylor's formula with the remainder depending on the second order differential: for any $x \in S$ there exists a point ξ_x belonging to the segment with endpoints x and $\overline{p}$ such that

$$f(x) - f(\overline{p}) - df(\overline{p})(x-\overline{p}) = \frac{1}{2}d^2f(\xi_x)(x-\overline{p}, x-\overline{p}). \tag{4}$$

Since the left–hand side is an integrable function of $x \in S$, then so is the right–hand side. Observe that $x \mapsto df(\overline{p})(x-\overline{p})$ is an affine function, whence by Lemma 1

$$\int_S df(\overline{p})(x-\overline{p})dx = df(\overline{p})(\overline{p}-\overline{p}) = 0.$$

Therefore integrating both sides of (4) and using (3) we get

$$\begin{aligned}\left|\int_S f(x)dx - \operatorname{vol}(S) f(\overline{p})\right| &= \frac{1}{2}\left|\int_S d^2f(\xi_x)(x-\overline{p}, x-\overline{p})dx\right| \\ &\leqslant \frac{1}{2}\int_S \left|d^2f(\xi_x)(x-\overline{p}, x-\overline{p})\right| dx \\ &\leqslant \frac{1}{2}\|d^2f\|_\infty \int_S \|x-\overline{p}\|^2 dx.\end{aligned}$$

□

THEOREM 7. *Let $\mathscr{T}$ be a positive linear functional defined on $\mathscr{C}^2(S)$ such that $\mathscr{T}(p) = \int_S p(x)dx$ for all polynomials $p : \mathbb{R}^n \to \mathbb{R}$ of degree at most 2. Then*

$$\left|\int_S f(x)dx - \mathscr{T}(f)\right| \leqslant \|d^2f\|_\infty \int_S \|x-\overline{p}\|^2 dx$$

for any $f \in \mathscr{C}^2(S)$.

Proof. Let $g(x) = \frac{\|d^2f\|_\infty}{2}\|x\|^2$, $x \in S$. By Lemma 5 the functions $g+f$ and $g-f$ are convex. Observe that the operator $\frac{1}{\operatorname{vol}(S)}\mathscr{T}$ fulfils the assumptions of Theorem 2 (for the purposes of this proof it is enough to have $\mathscr{T}$ defined on $\mathscr{C}^2(S)$, the assertion of Theorem 2 holds also in this setting). Then

$$\operatorname{vol}(S)(g+f)(\overline{p}) \leqslant \mathscr{T}(g+f) \quad \text{and} \quad \operatorname{vol}(S)(g-f)(\overline{p}) \leqslant \mathscr{T}(g-f).$$

Using the first of the above inequalities, Lemma 6 and the second assertion of Lemma 5 we infer that

$$\begin{aligned} \int_S (g+f)(x)dx &\leqslant \operatorname{vol}(S)\big(g(\overline{p})+f(\overline{p})\big) + \frac{1}{2}\big\|d^2(g+f)\big\|_\infty \int_S \|x-\overline{p}\|^2 dx \\ &\leqslant \mathscr{T}(g+f) + \|d^2 f\|_\infty \int_S \|x-\overline{p}\|^2 dx. \end{aligned}$$

Since $\int_S g(x)dx = \mathscr{T}(g)$, then

$$\int_S f(x)dx - \mathscr{T}(f) \leqslant \|d^2 f\|_\infty \int_S \|x-\overline{p}\|^2 dx. \tag{5}$$

Repeating the above argument for $g-f$ we arrive at

$$-\left[\int_S f(x)dx - \mathscr{T}(f)\right] \leqslant \|d^2 f\|_\infty \int_S \|x-\overline{p}\|^2 dx,$$

which, together with (5), finishes the proof. □

To approximately compute multiple integrals on simplices using the cubature rules it is enough to have error bounds of such rules on the unit simplex S_1, i.e. on the simplex with vertices $(0,0,\dots,0)$, $(1,0,\dots,0)$, $(0,1,\dots,0)$, …, $(0,0,\dots,1)$. The integral over any simplex by the appropriate affine variable interchange can be computed as an integral over S_1. That is why we record below the following

COROLLARY 8. *Let $\mathscr{T}$ be a positive linear functional defined on $\mathscr{C}^2(S_1)$ such that $\mathscr{T}(p) = \int_{S_1} p(x)dx$ for all polynomials $p:\mathbb{R}^n \to \mathbb{R}$ of degree at most 2. Then*

$$\left|\int_{S_1} f(x)dx - \mathscr{T}(f)\right| \leqslant \frac{n^2}{(n+2)!(n+1)}\|d^2 f\|_\infty$$

for any $f \in \mathscr{C}^2(S_1)$.

Proof. To prove the Corollary by Theorem 7 it is enough to check that

$$\int_{S_1} \|x-\overline{p}\|^2 dx = \frac{n^2}{(n+2)!(n+1)}, \quad \text{where } \overline{p} = \left(\frac{1}{n+1},\dots,\frac{1}{n+1}\right).$$

For $x=(x_1,\dots,x_n) \in S_1$ we have

$$\begin{aligned} \|x-\overline{p}\|^2 &= \sum_{i=1}^n \left[x_i - \frac{1}{n+1}\right]^2 = \sum_{i=1}^n \left[x_i^2 - \frac{2}{n+1}x_i + \frac{1}{(n+1)^2}\right] \\ &= \sum_{i=1}^n \left[\pi_i^2(x) - \frac{2}{n+1}\pi_i(x) + \frac{1}{(n+1)^2}\right], \end{aligned}$$

where $\pi_i(x) = x_i$ is the projection to the i–th axis. It is well known that $\operatorname{vol}(S_1) = \frac{1}{n!}$. Bessenyei [1, Lemma 1] computed

$$\int_{S_1} \pi_i(x)dx = \frac{1}{(n+1)!}, \quad i = 1, \ldots, n.$$

Repeating his argument we can easily compute

$$\int_{S_1} \pi_i^2(x)dx = \frac{2}{(n+2)!}, \quad i = 1, \ldots, n.$$

Then

$$\begin{aligned}
\int_{S_1} \|x-\overline{p}\|^2 dx &= \sum_{i=1}^{n} \int_{S_1} \left[\pi_i^2(x) - \frac{2}{n+1}\pi_i(x) + \frac{1}{(n+1)^2} \right] dx \\
&= \sum_{i=1}^{n} \left[\frac{2}{(n+2)!} - \frac{2}{n+1} \cdot \frac{1}{(n+1)!} + \frac{1}{(n+1)^2} \cdot \frac{1}{n!} \right] \\
&= n \left[\frac{2}{(n+2)!} - \frac{1}{(n+1)!} \cdot \frac{1}{(n+1)} \right] = \frac{n^2}{(n+2)!(n+1)}.
\end{aligned}$$

□

The above Corollary is useful in the approximate integration since an important class of positive linear functionals which coincide with the integral for polynomials of degree at most 2 are operators of the form of a conical combination of some values of an integrand at appropriately chosen points. Below we give an example of such cubature operator.

COROLLARY 9. *Let T be the unit simplex in $\mathbb{R}^2$,*

$$\mathscr{T}(f) := \frac{1}{24}\big(f(0,0) + f(0,1) + f(1,0)\big) + \frac{3}{8} f\left(\frac{1}{3}, \frac{1}{3}\right).$$

Then

$$\left| \iint_T f(x,y)dxdy - \mathscr{T}(f) \right| \leqslant \frac{1}{18} \|d^2 f\|_\infty$$

for any $f \in \mathscr{C}^2(T)$.

Proof. A cubature operator $\mathscr{T}$ fulfils all the assumptions of Corollary 8, in particular, $\mathscr{T}(p) = \iint_T p(x,y)dxdy$ for any polynomial $p : \mathbb{R}^2 \to \mathbb{R}$ of degree at most 2. □

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