



# Sharp Multidimensional Numerical Integration for Strongly Convex Functions on Convex Polytopes

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**Abstract.** This paper introduces and studies a new class of multidimensional numerical integration, which we call “strongly positive definite cubature formulas”. We establish, among others, a characterization theorem providing necessary and sufficient conditions for the approximation error (based on such cubature formulas) to be bounded by the approximation error of the quadratic function. This result is derived as a consequence of two characterization results, which are of independent interest, for linear functionals obtained in a more general setting. Thus, this paper extends some result previously reported in [2, 3] when convexity in the classical sense is only assumed. We also show that the *centroidal Voronoi Tessellations* provide an efficient way for constructing a class of optimal of cubature formulas. Numerical results for the two-dimensional test functions are given to illustrate the efficiency of our resulting cubature formulas.

## 1. Introduction and motivation for the problem

We introduce and study a class of a new class of multidimensional numerical integrations, that underestimate the exact value of the integral of every strongly convex function. For brevity, we call them “strongly positive definite cubature formulas” (or for short spd-formulas). These provide a natural generalization of some results presented in [2, 3] to the setting where the integrands are strongly convex. Let us mention that all the papers [2, 3] are derived in the context of convexity in the classical sense. Our first main results, which hold in large generality and are of independent interest, concern two characterization results of any linear functional  $C^{1,1}(\Omega) \rightarrow \mathbb{R}$ , which is nonnegative on the set of convex functions. These results, which find applications in the later sections, are stated in Section 2. In Section 3, we first apply our general results to the case when the functional is the error functional of spd-formulas. It is shown that, for functions belonging to  $C^{1,1}(\Omega)$ , the absolute value of the approximation error based on such cubature formulas can be bounded by the approximation error of the quadratic function. In addition, for integrands which satisfy the classical convexity or, more generally, strong convexity, we derive sharp upper and also lower bounds for the approximation error. We also propose two methods for their constructions. The first one is given in terms of the partition of unity of the integration domain. However, the second one is based on a decomposition method for domain integration. In section 4, we derive optimal global error estimates and also show that the centroidal Voronoi tessellations give access to efficient algorithms for constructing such cubature formulas. Finally, Section 5 provides two numerical examples to validate our approach.

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## 2. Notation, terminology and preliminary results

We first introduce some notations, which follow closely those of [2, 3]. The set of all positive real numbers is denoted by  $\mathbb{R}^+$ . Let  $\Omega$  be a subset of  $\mathbb{R}^d$ . We denote by  $\|\cdot\|$  the Euclidean norm in  $\mathbb{R}^d$  and  $\langle \mathbf{x}, \mathbf{y} \rangle$  the standard inner product of  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ . By  $C^{1,1}(\Omega)$  we denote the class of all functions  $f$  which are continuously differentiable on  $\Omega$  with Lipschitz continuous gradients, i.e., there exists  $L(\nabla f)$  such that

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L(\nabla f) \|\mathbf{x} - \mathbf{y}\|, \quad (\mathbf{x}, \mathbf{y} \in \Omega).$$

A convex function  $f$  is said to be  $\mu$ -strongly convex function if, and only if, there exists a constant  $\mu \geq 0$  such that the function  $f - \frac{\mu}{2} \|\cdot\|^2$  is convex.

A linear functional  $R : C(\Omega) \rightarrow \mathbb{R}$  is positive on  $X \subset C(\Omega)$  if and only if  $R(f) \geq 0$  whenever  $f \in X$ . Let  $CC(\Omega)$  denote the set of all continuous convex functions on  $\Omega$ , and  $SC_\mu(\Omega)$  the set of all  $\mu$ -strongly continuous convex functions on  $\Omega$ .

We start by providing two characterization results for any linear functional, which hold in large generality and is of independent interest. But to apply our approach, we are mainly interested here in the case when the functional  $R$  is the approximation error of our cubature formulas. These results will be important in the sequel. The first general characterization result is given in the following:

**Lemma 2.1** *Let  $\mu > 0$  and  $\Omega \subset \mathbb{R}^d$  be a compact convex set. Let  $R : C(\Omega) \rightarrow \mathbb{R}$ , be a linear functional. Then,  $R$  is positive on  $CC(\Omega)$  if and only is  $R$  is positive on  $SC_\mu(\Omega)$ .*

*Proof.* It suffices to show that any positive linear function on  $SC_\mu(\Omega)$  is also positive on  $CC(\Omega)$  because  $SC_\mu(\Omega)$  is a subset of  $CC(\Omega)$ . Let us assume that  $R$  is positive on  $SC_\mu(\Omega)$  and take any  $f \in CC(\Omega)$ . Define

$$g := f + \frac{\varepsilon}{2} \|\cdot\|^2.$$

Multiplying by  $\frac{\mu}{\varepsilon}$  and rearranging, we deduce

$$\frac{\mu}{\varepsilon} f = \frac{\mu}{\varepsilon} g - \frac{\mu}{2} \|\cdot\|^2.$$

Since  $\frac{\mu}{\varepsilon} f$  is convex, then  $\frac{\mu}{\varepsilon} g$  is  $\mu$ -strongly convex. Now, from the positivity of  $R$  on  $SC_\mu(\Omega)$ , it follows

$$R\left(\frac{\mu}{\varepsilon} g\right) \geq 0.$$

Hence, the homogeneity of  $R$  implies

$$R(g) \geq 0.$$

Hence, the linearity of  $R$  yields :

$$R(f) \geq -\frac{\varepsilon}{2} R(\|\cdot\|^2).$$

Since this inequality holds for all  $\varepsilon > 0$ , then by letting  $\varepsilon \downarrow 0$ , we get

$$R(f) \geq 0.$$

Hence, the desired result follows.  $\square$

Under regularity conditions, the functions belong to  $C^{1,1}(\Omega)$ , our second characterization result is given in the following:

**Lemma 2.2** Let  $\Omega \subset \mathbb{R}^d$  be a compact convex set. Let  $\mu > 0$  and  $R : C^k(\Omega) \rightarrow \mathbb{R}$ , where  $k \in \{0, 1\}$ , be a linear functional. Then  $R$  is positive on  $SC_\mu(\Omega) \cap C^{1,1}(\Omega)$  if and only if for every  $f \in C^{1,1}(\Omega)$ , it holds

$$|R[f]| \leq \frac{L[\nabla f]}{2} R[\|\cdot\|^2], \tag{1}$$

where  $L[\nabla f]$  is the Lipschitz parameter of the gradient of  $f$ .

*Proof.* Let us assume that  $R$  is positive on  $SC_\mu(\Omega) \cap C^{1,1}(\Omega)$  and take any function  $f$  from  $C^{1,1}(\Omega)$ . Define the two following functions

$$h_\pm := \frac{L[\nabla f]}{2} \|\cdot\|^2 \pm f.$$

Then, [3, proposition 2.2] tells us that  $h_\pm \in CC(\Omega) \cap C^{1,1}(\Omega)$ . Hence, by application of Lemma 2.1, we may conclude that

$$R[h_\pm] \geq 0.$$

Then, by linearity of  $R$  and a simple manipulation we find that

$$-\frac{L[\nabla f]}{2} R[\|\cdot\|^2] \leq R[f] \leq \frac{L[\nabla f]}{2} R[\|\cdot\|^2].$$

This shows that (1) is satisfied.

Now, let us assume that (1) holds. Then, (1) obviously implies

$$R[\|\cdot\|^2] \geq 0, \tag{2}$$

and that

$$R\left[\frac{L[\nabla f]}{2} \|\cdot\|^2 - f\right] \geq 0. \tag{3}$$

For any  $h \in SC_\mu(\Omega) \cap C^{1,1}(\Omega)$  define

$$f := \frac{L[\nabla h]}{2} \|\cdot\|^2 - h.$$

Then, in view of [3, proposition 2.2], once again we get

$$f \in C^{1,1}(\Omega) \text{ and } L[\nabla h] - L[\nabla f] \geq 0. \tag{4}$$

But, since

$$h = \frac{L[\nabla h]}{2} \|\cdot\|^2 - f,$$

it can be written as follows

$$h = \left(\|\cdot\|^2 \frac{L[\nabla f]}{2} - f\right) + \frac{L[\nabla h] - L[\nabla f]}{2} \|\cdot\|^2,$$

we therefore obtain

$$R[h] = R\left[\|\cdot\|^2 \frac{L[\nabla f]}{2} - f\right] + \frac{L[\nabla h] - L[\nabla f]}{2} R[\|\cdot\|^2].$$

Finally, this together (2), (3) and (4) yield the desired result  $R[h] \geq 0$ .  $\square$

### 3. Spd-cubature formulas

We now define our new general class of cubature formulas:

**Definition 3.1** Let  $\Omega$  be a compact subset of  $\mathbb{R}^d$  and let  $\mu > 0$ . Let  $x_1, \dots, x_n \in \Omega$ , and  $\omega_1, \dots, \omega_n \in \mathbb{R}^+$ . We say that

$$\{(\omega_i, x_i) : i = 1, \dots, n\}, \tag{5}$$

defines the  $\mu$  spd-cubature formula

$$\int_{\Omega} f(x) dx = \sum_{i=1}^n \omega_i f(x_i) + R[f], \tag{6}$$

if the approximation error  $R$  is positive on  $SC_{\mu}(\Omega)$ .

Now, the general results derived in Lemmas 2.1 and 2.2 can be applied to the approximation error of our class of cubature formulas to characterize it as follows:

**Theorem 3.2** let  $\mu > 0$  and let  $\Omega$  be a compact subset of  $\mathbb{R}^d$ . A cubature formula (6) is  $\mu$  spd-formula if and only if for all  $f \in C^{1,1}(\Omega)$ , its approximation error satisfies

$$\frac{\mu}{2} R[\|\cdot\|^2] \leq R[f] \leq \frac{L[\nabla f]}{2} R[\|\cdot\|^2]. \tag{7}$$

### 4. Global error estimates

In this section, we derive optimal global error estimates and also show that the centroidal Voronoi diagrams give access to efficient algorithms for constructing such cubature formulas. Let  $\Omega \subset \mathbb{R}^d$  be a polytope and let  $\mathcal{D}$  be a decomposition of  $\Omega$ . Here the integration domain  $\Omega$  is decomposed into a disjoint union of open convex subpolytopes  $\Omega = \bigcup_{P \in \mathcal{D}} P$ . Since

$$\int_{\Omega} f(x) dx = \sum_{P \in \mathcal{D}} \int_P f(x) dx$$

it produces the cubature formulas

$$\int_{\Omega} f(x) dx = \sum_{P \in \mathcal{D}} Q_P^{\text{mid}}(f) + E_{\Omega}^{\text{mid}}(f), \tag{8}$$

where the cubature formulas  $Q_P^{\text{mid}}$  is given by

$$Q_P^{\text{mid}}(f) = |P| f(c_P), \tag{9}$$

here  $c_P$  is the the center of gravity of  $P$ . The resulting cubature formula  $\sum_{P \in \mathcal{D}} Q_P^{\text{mid}}(f)$  is a *spd*-cubature formula. The following result is a simple consequence of Theorems 3.2.

**Theorem 4.1** Let  $f \in C^{1,1}(\Omega)$  with  $L[\nabla f]$ -Lipschitz constant. Let the cubature formula be given as in (8). Then, the following error estimate holds:

$$|E_{\Omega}^{\text{mid}}(f)| \leq \frac{L[\nabla f]}{2} \sum_{P \in \mathcal{D}} \int_P \|x - c_P\|^2 dx. \tag{10}$$

In order to minimize the energy functional

$$F_E = \sum_{P \in \mathcal{D}} \int_P \|x - c_P\|^2 dx, \tag{11}$$

which correlates with the upper bounds of approximation errors, see Theorem 4.1, we first present the definition and properties of the *Centroidal Voronoi Tessellations (CVT)*. The reader requiring more information on the subject is referred to the survey paper [1]. Given  $k$  points  $x_1, x_2, \dots, x_k$  inside the polytope  $\Omega$ , the Voronoi diagram is defined as the collection of the Voronoi regions  $\Omega_i, i = 1, 2, \dots, k$ , that are defined as

$$\Omega_i = \{x \in \Omega : \|x - x_i\| < \|x - x_j\|, j \neq i\}.$$

The CVT is a special Voronoi diagram in which each generator point  $x_i$  coincides with the center of gravity  $s_{\Omega_i}$  of its Voronoi region

$$x_i = s_{\Omega_i} = \frac{\int_{\Omega_i} x dx}{\int_{\Omega_i} \mu(x) dx}.$$

It is well known that a necessary condition for minimizing (11) is that  $\mathcal{D}$  is a CVT with generators  $\{s_{\Omega_i}, \Omega_i \in \mathcal{D}\}$ , see [1, Proposition 3.1]. Theorem 4.1 gives the constructive way for building cubature formulas with the best global error estimates. To this end one should construct CVT and then apply the formula  $Q_{\Omega}^{\text{mid}}$ .

### 5. Numerical Examples

In order to validate our approach, we next consider the two following bivariate test functions:

$$f_1(x) = \exp(\alpha x + \beta y), \quad \alpha, \beta \in \mathbb{R}, \tag{12}$$

$$f_2(x) = y \arctan(\alpha(x + y)), \quad \alpha \in \mathbb{R}^+, \tag{13}$$

where  $x = (x, y) \in [-1, 1] \times [-1, 1]$ . These two functions are infinitely differentiable, they have singularities or large gradients, when  $\alpha$  and  $\beta$  are sufficiently large enough, see Figure 1.

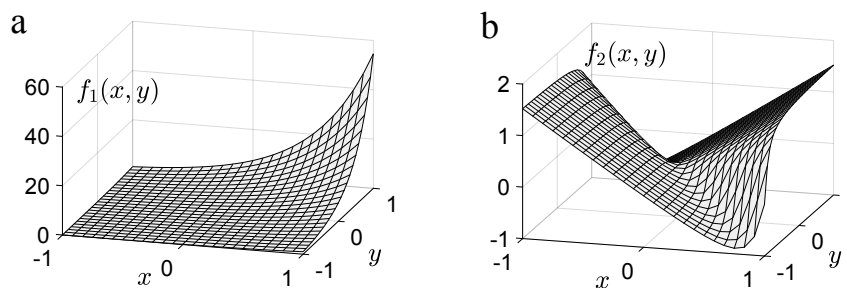


Figure 1: Test functions: (a)  $f(x, y)$  for the case  $\alpha = \beta = 2$  and (b)  $g(x, y)$  for  $\alpha = 10$ .

The exact values of their integrals of over  $\Omega := [-1, 1] \times [-1, 1]$  are given by

$$I(f) = \frac{4 \sinh(\alpha) \sinh(\beta)}{\alpha \beta},$$

$$I(g) = -\frac{8\alpha^2 - 2\alpha(3 + 4\alpha^2) \arctan(2\alpha) + \log(1 + 4\alpha^2)}{6\alpha^3}.$$

All the integrals are approximated using cubature formulas  $Q_{\Omega}^{\text{mid}}(h)$ , see (8). We used CVT generated by original PolyMesher, see [4]. Here  $N$  is the square root of the number of Voronoi regions, and  $\Omega_i$  is the Voronoi region,  $i = 1, \dots, N^2$ . We denote the resulting cubature formula by  $Q_N^{\text{mid}}(f)$ .

Let  $E_N^{\text{mid}}(f)$  denote the relative error associated to  $Q_N^{\text{mid}}(h)$

$$E_N^{\text{mid}}(h) = \frac{Q_N^{\text{mid}}(h) - I(h)}{I(h)}, \quad h \in \{f, g\}. \tag{14}$$

The following figure shows the corresponding mesh of the centroidal Voronoi cubature formula  $Q_N^{\text{mid}}$ .

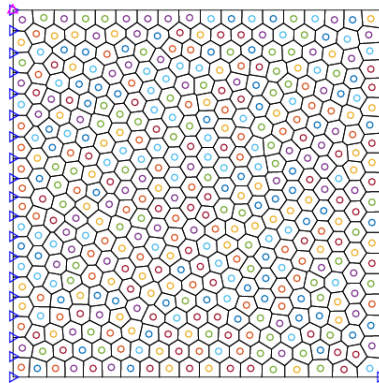


Table 1: The CVT and its generators of the unit square, here  $N = 20$ .

Table 2 shows the relative errors for the test function  $f(x)$  for the fixed parameters  $\alpha = \beta = 1$ . Table 3 shows the orders of convergence.

$N$	4	8	16	32	64	128	256
$E_N^{\text{mid}}(f)$	2.2E-02	4.31E-03	1.35E-03	3.25E-04	7.99E-05	1.99E-05	4.98E-06

Table 2: Approximation errors of integration for the test function  $f(x)$  with parameters  $\alpha = \beta = 1$

$N$	8	16	32	64	128	256
$E_N^{\text{mid}}(f)$	2.0959	1.9821	1.9723	2.0124	2.0022	1.981

Table 3: Orders of convergence for the test function  $f(x)$  with parameters  $a = b = 1$ .

Finally, Table 4 and Table 5 show, respectively, the relative errors and orders of convergence for test function  $g(x)$  with parameter  $\alpha = 1$ .

$N$	4	8	16	32	64	128	256
$E_N^{\text{mid}}(g)$	8.64E-02	.46E-02	3.61E-03	9.95E-04	2.45E-04	6.07E-05	1.52E-05

Table 4: A pproximation errors for the test function  $g(x)$  with parameter  $a = 1$

$N$	8	16	32	64	128	256
$E_N^{\text{mid}}(g)$	2.5621	2.0194	1.859	2.0227	2.0125	1.993

Table 5: Orders of convergence for the test function  $g(x)$  with parameter  $a = 1$ .

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