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par

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**Approximation of multivariate functions under certain generalized
convexity assumptions**

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applications (LMAP) à Pau**

Dedication

This dissertation work is dedicated to:

- **My dearest mother for being the first teacher in my life (God bless her soul and may she rest in peace)**
- **My father for earning an honest living for us and for supporting and encouraging me to believe in myself**
- **My sweetheart my wife (Lobna), who leads me through the valley of darkness with light of hope and support**
- **My beloved kid (Ibrahim)**
- **My beloved brothers and sister (Ammar, Mustafa, Muna)**
- **My friends who encourage and support me**
- **My homeland (IRAQ) and all the people in my life who touch my heart.**



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Abstract

In many applications, we may wish to interpolate or approximate a multivariate function possessing certain geometric properties or “shapes” such as smoothness, monotonicity, convexity or nonnegativity. These properties may be desirable for physical (e.g., a volume-pressure curve should have a nonnegative derivative) or practical reasons where the problem of shape preserving interpolation is important in various problems occurring in industry (e.g., car modelling, construction of mask surface). Hence, an important question arises: How can we compute the best possible approximation to a given function f when some of its additional characteristic properties are known?

This thesis presents several new techniques to find a good approximation of multivariate functions by a new kind of linear operators, which approximate from above (or, respectively, from below) all functions having certain generalized convexity. We focus on the class of convex and strongly convex functions. We would wish to use this additional information in order to get a good approximation of f . We will describe how this additional condition can be used to derive sharp error estimates for continuously differentiable functions with Lipschitz continuous gradients. More precisely we show that the error estimates based on such operators are always controlled by the Lipschitz constants of the gradients, the convexity parameter of the strong convexity and the error associated with using the quadratic function. Assuming, in addition, that the function, we want to approximate, is also strongly convex, we establish sharp upper as well as lower refined bounds for the error estimates.

Approximation of integrals of multivariate functions is a notoriously difficult tasks and satisfactory error analysis is far less well studied than in the univariate case. We propose a method to approximate the integral of a given multivariate function by cubature formulas (numerical integration), which approximate from above (or from below) all functions having a certain type of convexity. We shall also see, as we did for for approximation of functions, that for such integration formulas, we can establish a characterization result in terms of sharp error estimates. Also, we investigated the problem of approximating a definite integral of a given function when a number of integrals of this function over certain hyperplane sections of d -dimensional hyper-rectangle are only available rather than its values at some points.

The motivation for this problem is multifold. It arises in many applications, especially in experimental physics and engineering, where the standard discrete sample values from functions are not available, but only their mean values are accessible. For instance, this data type

Abstract (English)

appears naturally in computer tomography with its many applications in medicine, radiology, geology, amongst others.

Résumé

Dans de nombreuses applications, nous souhaitons interpoler ou approcher une fonction de plusieurs variables possédant certaines propriétés ou “formes” géométriques, telles que la régularité, la monotonie, la convexité ou la non-négativité. Ces propriétés sont importantes pour des applications en physique (par exemple, la courbe pression-volume doit avoir une dérivée non négative), aussi bien où le problème de l’interpolation conservant la forme est essentiel dans divers problèmes de l’industrie (par exemple, modélisation automobile, construction de la surface du masque). Par conséquent, une question importante se pose : comment calculer la meilleure approximation possible à une fonction donnée f lorsque certaines de ses propriétés caractéristiques supplémentaires sont connues ?

Cette thèse présente plusieurs nouvelles techniques pour trouver une bonne approximation des fonctions de plusieurs variables par des opérateurs linéaires dont l’erreur d’approximation $A(f) - f$ garde un signe constant pour toute fonction f satisfaisant une certaine convexité généralisée. Nous nous concentrons dans cette thèse sur la classe des fonctions convexes ou fortement convexes. Nous décrivons comment la connaissance a priori de cette information peut être utilisée pour déterminer une bonne majoration de l’erreur pour des fonctions continuellement différentiables avec des gradients Lipschitz continus. Plus précisément, nous montrons que les estimations d’erreur basées sur ces opérateurs sont toujours contrôlées par les constantes de Lipschitz des gradients, le paramètre de la convexité forte ainsi que l’erreur commise associée à l’utilisation de la fonction quadratique. En supposant en plus que la fonction que nous voulons approcher est également fortement convexe, nous établissons de meilleures bornes inférieures et supérieures pour les estimations d’erreur de l’approximation. Les méthodes de quadrature multidimensionnelle jouent un rôle important, voire fondamental, en analyse numérique. Une analyse satisfaisante des erreurs provenant de l’utilisation des formules de quadrature multidimensionnelle est bien moins étudiée que dans le cas d’une variable. Nous proposons une méthode d’approximation de l’intégrale d’une fonction réelle donnée à plusieurs variables par des formules de quadrature, qui conduisent à des valeurs approchées par excès (respectivement par défaut) des intégrales des fonctions ayant un certain type de convexité. Nous verrons aussi, comme nous l’avons fait pour l’approximation des fonctions, que pour de telles formules d’intégration, on peut établir un résultat de caractérisation en termes d’estimations d’erreur. En outre, nous avons étudié le problème de l’approximation d’une intégrale définie d’une fonction donnée quand un certain nombre d’intégrales de cette fonction sur certaines sections hyperplanes d’un l’hyper-rectangle sont seulement disponibles.

La motivation derrière ce type de problème est multiple. Il se pose dans de nombreuses applications, en particulier en physique expérimentale et en ingénierie, où les valeurs standards des échantillons discrets des fonctions ne sont pas disponibles, mais où seulement leurs valeurs moyennes sont accessibles. Par exemple, ce type de données apparaît naturellement dans la tomographie par ordinateur avec ses nombreuses applications en médecine, radiologie, géologie, entre autres.

Contents

Acknowledgements	i
Abstract (English)	iii
Résumé (Français)	v
Table of contents	vii
List of figures	xi
List of tables	xv
Notations	xvii

General Introduction	1
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Introduction générale (Français)	5
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their Generalizations	11
1.1 Usual convexity	11
1.1.1 Notation and Terminology	11
1.1.2 Convex functions of one variable	12
1.1.3 Convex sets	13
1.1.4 Multivariate convex functions	15
1.1.5 Characterizations of convexity	23
1.2 Strong convexity and its characterizations	27
1.2.1 Characterizations in terms of usual convexity	29
1.2.2 Uniqueness of minimum for strongly convex functions	30
1.2.3 The first-order condition for strongly convex functions	31
1.2.4 Characterization via the strong monotonicity of the gradient	33
1.2.5 The second-order condition for strongly convex functions	35
1.3 Convex functions with Lipschitz continuous gradients	36
1.3.1 Lipschitz-continuous gradient	36
1.3.2 Sandwiching smooth convex functions	38
1.3.3 Error estimates for linear approximation	39
1.3.4 Characterization of Lipschitz continuity of the gradient	39

Contents

1.3.5 Strong convex functions with Lipschitz continuous derivatives	40
1.3.6 Co-coercivity property for strongly convex functions	41
Bibliography	43
2 Approximations of differentiable convex functions on arbitrary convex polytopes	45
2.1 Convex polytopes	45
2.1.1 Fundamental theorems and properties of polytopes	48
2.2 Barycentric coordinates	49
2.2.1 Generalized barycentric coordinates on polytopes	50
2.3 Approximations of differentiable convex functions on arbitrary convex polytopes	55
Bibliography	63
3 On the approximation of strongly convex functions by an upper or lower operator	67
3.1 Some background and motivation	67
3.2 Characterizations of upper or lower approximation operators	71
3.3 Applications to the barycentric approximation schemes	74
3.4 Numerical experiments	78
3.5 Numerical examples and MSE error	80
Bibliography	83
4 Numerical integration under certain type of convexity	85
4.1 Notation, Terminology and preliminary results	86
4.2 Strongly positive definite cubature formulas	90
4.2.1 Construction and Characterization of Strongly Positive Definite Cubature Formulas	90
4.3 Strongly Negative Definite Cubature Formulas	95
4.3.1 Characterization of Strongly Negative Definite Cubature Formulas	96
4.3.2 Practical Construction of Strongly Negative Definite Cubature Formulas	98
4.4 Numerical Examples	99
Bibliography	107
5 New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d-dimensional hyper-rectangle	109
5.1 Introduction	110
5.2 A multivariate version of the trapezoidal rule	114
5.3 A multivariate version of the midpoint rule	117
5.4 Average cubature formulas	119
5.5 A multivariate version of perturbed midpoint, trapezoidal, and Simpson's rule	121
5.6 Cubature Error Bounds	125
5.7 Numerical tests	128

Bibliography	139
Conclusion and final remarks (English)	141
Conclusion et remarques finales (Français)	143

List of Figures

1.1	illustration of the inequality $f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda)f(y)$	13
1.2	Any minimum of convex function is a global minimum.	15
1.3	non-global local minimal.	16
1.4	convex function.	16
1.5	convex function.	17
1.6	concave function.	17
1.7	concave function.	18
1.8	neither convex nor concave.	18
1.9	neither convex nor concave.	19
1.10	convex and concave.	19
1.11	If f is convex and differentiable, then $f(x) \leq hf(x, (y-x)) \leq f(y)$ for all x, y belonging to domain of f (the first order characteristic of a convex function).	25
1.12	If f is convex and differentiable, then $f(x) \leq hf(x, (y-x)) \leq f(y)$ for all x, y belonging to domain of f (the first order characteristic of a convex function).	25
2.1	6-gon or hexagon.	46
2.2	the tetrahedron in $\mathbb{R}^3$	47
2.3	Polytope which presented in two ways either as a $\mathbb{R}^n$ polytope or as an H polytope.	47
2.4	Every triangle in a Delaunay triangulation has an empty open circumdisk. . .	53
2.5	Delaunay triangles and edges whose interiors intersect.	54
2.6	Voronoi diagram.	55
2.7	Voronoi diagram.	55
3.1	The figure on the left shows the graph of f produced by MAPLE, and using MATLAB the graph on the right is for the piecewise-linear interpolation of the data generated from f	79
3.2	The figure on the left shows the graph of f_1 and the graph on the right for the piecewise-linear interpolation of the data generated from f_1	81
3.3	The figure on the left shows the graph of f_2 and the graph on the right for the piecewise-linear interpolation of the data generated from f_2	81
4.1	Illustrate the error generated from using cubature formula to approximate the integral of f_1	102

List of Figures

4.2	Illustrate the error generated from using cubature formula to approximate the integral of f_1 in the log scale.	102
4.3	Illustrate the error generated from using cubature formula to approximate the integral of f_2	103
4.4	Illustrate the error generated from using cubature formula to approximate the integral of f_2 in the log scale.	103
4.5	Illustrate the error generated from using cubature formula to approximate the integral of f_3	104
4.6	Illustrate the error generated from using cubature formula to approximate the integral of f_3 in the log scale.	104
4.7	Illustrate the error of numerical integration for function f_1 and linear regression.	105
4.8	Illustrate the error of numerical integration for function f_2 and linear regression.	105
4.9	Illustrate the error of numerical integration for function f_3 and linear regression.	106
5.1	Mesh of the unit square corresponding to the uniform centroidal Voronoi cubature formula (left), and that corresponding to the non-uniform centroidal Voronoi cubature formula (right). $N \approx 20$ in these examples.	130
5.2	Graph of the error corresponding to the approximation with the non-uniform centroidal Voronoi formula (left), and the error in the log scale (right).	130
5.3	Graph of the error corresponding to the approximation with the uniform centroidal Voronoi formula (left), and the error in the log scale (right).	131
5.4	Graph of the error corresponding to the approximation with the Trapezoidal formula (left), and the error in the log scale (right).	131
5.5	Graph of the error corresponding to the approximation with the Midpoint formula (left), and the error in the log scale (right).	132
5.6	Graph of the error corresponding to the approximation with the Hammer formula (left), and the error in the log scale (right).	132
5.7	Graph of the error corresponding to the approximation with the Simpson formula (left), and the error in the log scale (right).	133
5.8	Graph of the error corresponding to the approximation of each formula (left), and the error in the log scale (right).	133
5.9	Graph of the error corresponding to the approximation with the non-uniform centroidal Voronoi formula (left), and the error in the log scale (right).	135
5.10	Graph of the error corresponding to the approximation with the uniform centroidal Voronoi formula (left), and the error in the log scale (right).	135
5.11	Graph of the error corresponding to the approximation with the Trapezoidal formula (left), and the error in the log scale (right).	136
5.12	Graph of the error corresponding to the approximation with the Midpoint formula (left), and the error in the log scale (right).	136

- 5.13 Graph of the error corresponding to the approximation with the Hammer formula (left), and the error in the log scale (right). 137
- 5.14 Graph of the error corresponding to the approximation with the Simpson formula (left), and the error in the log scale (right). 137
- 5.15 Graph of the error corresponding to the approximation of each formula (left), and the error in the log scale (right). 138

List of Tables

3.1 MSE for a function f_1	81
3.2 MSE for a function f_2	81
3.3 MSE for a function f_3	82
3.4 MSE for a function f_4	82
4.1 The error of numerical integration for function f_1	100
4.2 The error of numerical integration for function f_2	101
4.3 The error of numerical integration for function f_3	101
5.1 The behavior of the error corresponding to each cubature formula for the test function f_1	129
5.2 The behavior of the error corresponding to each cubature formula for the test function f_2	134

Notations

General notations

$\mathbf{R}$	the set of real numbers
$\mathbf{R}^{\geq 0}$	the set of all nonnegative real numbers
$\mathbf{R}^{\leq 0}$	the set of all nonpositive real numbers
$\mathbf{R}^{> 0}$	the set of all positive real numbers
$\mathbf{R}^d$	d -dimensional Euclidean space
$d\mathbf{R}^d$	the Euclidean distance in $\mathbf{R}^d$
$\mathbf{x} \in (x_1, x_2, \dots, x_d) \in \mathbf{R}^d$	element of $\mathbf{R}^d$
$\ \mathbf{x}\ _2 = \sqrt{x_1^2 + x_2^2 + \dots + x_d^2}$	the Euclidean norm of $\mathbf{x}$ in $\mathbf{R}^d$
$\langle \mathbf{x}, \mathbf{y} \rangle$	the usual scalar product of $\mathbf{x}$ and $\mathbf{y}$ on $\mathbf{R}^d$.
$[\mathbf{x}, \mathbf{y}]$	the line segment between $\mathbf{x}$ and $\mathbf{y}$, for $\mathbf{x}, \mathbf{y} \in \mathbf{R}^d$.
$\nabla f(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}(\mathbf{x}), \frac{\partial f}{\partial x_2}(\mathbf{x}), \dots, \frac{\partial f}{\partial x_d}(\mathbf{x}) \right)$	the gradient of f at $\mathbf{x}$
$\mathbf{H}^2 f(\mathbf{x})$	the Hessian matrix of f at $\mathbf{x}$ with the matrix elements given by $\mathbf{H}^2 f(\mathbf{x})_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{x}), i \in 1, \dots, d, j \in 1, \dots, d.$
$\mathcal{S}^1$	the set of all strongly convex functions with convexity parameter 1

Notations

S^1	the set of all continuously differentiable strongly convex functions with convexity parameter $\gamma \in 0$
$S^{1,1}$	the set of all γ -strongly convex continuously differentiable functions with Lipschitz-continuous gradients
$S_{\gamma,L}$	the set of all γ -strongly convex functions such that the gradient ∇f is Lipschitz continuous with Lipschitz constant L
$conv$	the convex hull of a finite point set
ext	the set of all extreme points of
$vert$	the set of all vertices of
Del, DT	Delaunay triangulation
$C^{1,1}$	the subclass of all functions which are continuously differentiable with Lipschitz continuous gradients
$a(\phi)$	any affine function
MSE	the mean square error
T	triangulation of a finite d -dimensional set or simplicial complex
int	the interior of
$ j-j $	measure of
$L^1(-)$	all Lebesgue integrable functions
a.e.	almost everywhere
$C(-)$	all real-valued continuous functions on
$C^k(-)$	all functions which are k times continuously differentiable, where $k \in \mathbf{N}$

$\mathcal{E}_R f$	the error of cubature formulas for numerical integration of function f
C_d	d -dimensional hyper-rectangle
$M(f)$	the midpoint rule
$T(f)$	the trapezoid rule
$E M(f)$	the error of the rule $M(f)$
$E T(f)$	the error of the rule $T(f)$
C_{d+1}	the $(d+1)$ -dimensional hyper-rectangle in $\mathbf{R}^{d+1}$
$F_1, \dots, F_{2d}$	the $2d$ facets of C_d
$ C_d $	the d -dimensional volume
$ F_i $	the $(d+1)$ -dimensional volume
$Q^{\text{tr}}(f)$	the trapezoidal cubature formula
$E^{\text{tr}}(f)$	the approximation error of the trapezoidal cubature formula
$Q^{\text{mid}}(f)$	the midpoint cubature formula
$E^{\text{mid}}(f)$	the approximation error of the midpoint cubature formula
$Q^{\text{av}}(f)$	the average cubature formulas
$E^{\text{Sim}}(f)$	the approximation error of the Simpson cubature formula
$E^{\text{mper}}(f)$	the approximation error of the perturbed midpoint cubature formula
$E^{\text{tper}}(f)$	the approximation error of the perturbed trapezoidal cubature formula

Notations

$Q^{\text{Ham}}(f)$	the Hammer cubature formula
$UCVC$	uniform centroidal Voronoi cubature formula
$CV C$	non-uniform centroidal Voronoi cubature formula
$E_{N^{tr,mid,Sim,Ham,UCVC,CVC}}$	the absolute value of the error of the $\{tr,mi d, Si m, H am,UCVC,CVC\}$ cubature formula respectively for some integer value of N , where N is the number of subdivisions in each direction



General Introduction

Motivation

The main purpose of this thesis is to find a good approximation of multivariate functions by a new kind of linear operators, which approximate from above (or from below) all functions having certain generalized convexity. We focus on the class of convex and strongly convex functions. Actually, approximating an arbitrary function f is, in general, very difficult to do, but we sometimes know beforehand that f satisfies some known structural and regularity properties. For example, it may be known that this function has some additional kind of convexity, therefore we would wish to use this information in order to get a good approximation of f . We will describe how this additional knowledge can be used to derive sharp error estimates for continuously differentiable functions with Lipschitz continuous gradients. More precisely we show that the error estimates based on such operators are always controlled by the Lipschitz constants of the gradients, the convexity parameter of the strong convexity and the error associated with using the quadratic function. Assuming the function, we want to approximate, is also strongly convex, we establish sharp upper as well as lower refined bounds for the error estimates.

Approximation of integrals of multivariate functions is a notoriously difficult task and satisfactory error analysis is far less well studied than in the univariate case. We propose a method to approximate the integral of a given real-valued function of multiple variables by cubature formulas (numerical integration), which approximate from above (or from below) all functions having a certain type of convexity. We shall also see, as we did for approximation of functions, that for such integration formulas, we can establish a characterization result in terms of sharp error estimates. Also, we investigated the problem of approximating a definite integral of a given function when a number of integrals of this function over certain hyperplane sections of d -dimensional hyper-rectangle are only available rather than its values at some points.

The motivation for this problem is multifold. It arises in many applications, especially in

experimental physics and engineering, where the standard discrete sample values from functions are not available, but only their mean values are accessible. For instance, this data type appears naturally in computer tomography with its many applications in medicine, radiology, geology, amongst others.

Outline

This thesis consists of five chapters. The first chapter introduces the usual convexity and its generalizations. It includes almost everything pertinent and essential characterization results for (possibly smooth) convex functions. It also provides a unifying framework for many times surprisingly short proofs using well-known characterizations of convexity for functions of one variable. One of the most important properties of the convex function is that the function always controls its first order (linear) Taylor approximation. Unfortunately, in general, it is still difficult to get better bounds on the error introduced by such an approximation if no additional information is available. Therefore, we need to extend the notion of classical convexity. We realized that the natural condition that we can impose on the function is to belong the class of strongly convex functions. Furthermore, we will establish an intimate relationship between usual convexity and strong convexity which helped us to establish some important characterizations of these kind of functions. It is also shown that under strong convexity type restrictions, we can obtain better lower and upper bounds in linear approximation than that from usual convexity. This is one of the main aims of this chapter. For this end, we consider the case when, in addition, the gradients are Lipschitz continuous. In this setting, we present some characterization theorems and also give more controlled and then improved error bounds than those obtained for ordinary convexity. It is worth mentioning in this chapter, we are try to provide more details in the proofs where it felt needed based on [1, 7, 8, 10].

In the second chapter, due to the urgent need for some concepts and characterization theorems for this study, we begin by giving two equivalent definitions of a prototype and then state some well-known fundamental theorems and properties of such a geometric object. After that, we define the notion of generalized barycentric coordinates with respect to an arbitrary set of points in $\mathbf{R}^d$, or equivalently, with respect to a (convex) polytope. We then show that such coordinates always exist for any given finite point set. This existence result is due to Kalman in the sixties [26, Theorem 2]. Moreover, this chapter introduces Delaunay triangulations as geometrically duals to Voronoi diagrams. We summarize basic properties of such widely-used triangulations. Under the convexity assumption, we also provide an approximation method, which we call it a barycentric approximation. This class of (linear) operators approximate all convex functions from above. Finally, we give a characterization result for these operators in terms of their error estimates. Such a characterization theorem is due to Guessab in his recent paper [2].

In the third chapter, we have proposed a convenient and practical method to approximate a given real-valued function of multiple variables by linear operators, which approximate all *strongly* convex functions from above (or from below). We have used this additional knowledge to derive sharp error estimates for continuously differentiable functions with Lipschitz continuous gradients. More precisely, we show that the error estimates based on such operators are always controlled by the Lipschitz constants of the gradients, the convexity parameter of strong convexity and the error associated with using the quadratic function, as we will see in theorems 3.2.1 and 3.2.3. Moreover, assuming the function, we want to approximate, is also strongly convex, we establish sharp upper as well as lower refined bounds for the error estimates, see Corollaries 3.2.2 and 3.2.4. As an application, we define and study a class of linear operators on an arbitrary polytope, which approximate strongly convex functions from above. Finally, we present a numerical example illustrating the proposed method. Actually, one of the main reasons that attracted our attention to such class of functions is that these latter are used widely in economic theory (see [1]), and are also central to optimization theory (see [2]). Indeed, in the framework of function minimization, this convexity notion has important and well-known implications.

In chapter four, we have expanded some results of the papers [1, 2, 3, 4] by introducing a new class of cubature formulas for numerical integration (or multidimensional quadrature), that approximate from above (or from below) the exact value of the integrals of every function having a certain type of convexity. First, we would like to mention that all these papers were established in the context of the classical notion of convexity. Here, our objective is to extend the ideas given there under certain types of generalized convexity. To this end, in this chapter, we first present some definitions, notations and then state two characterization results of any linear functional $C^{1,1}(-) \rightarrow \mathbf{R}$, which is nonnegative on the set of convex functions. Furthermore we define two new classes of cubature formulas, which we call them strongly positive, respectively negative, definite cubature formulas. We then apply our general results to the case when the functional is the error functional of our cubature formulas. More precisely, we show that, for functions belonging to $C^{1,1}(-)$, the error estimates based on such cubature formulas may always be controlled by the Lipschitz constants of the gradients, the different types of convexity and the error associated with using the quadratic function. In addition, knowing whether the function to be integrated satisfies the classical convexity or strong convexity, we establish sharp upper as well as lower refined bounds for the error estimates. One of the valuable results in this chapter is that, for strongly positive definite cubature formulas, we establish characterization results between them and the partition of unity of the integration domain, but also show how we can construct them using the decomposition method for domain integration. The same thing has been done for strongly negative definite cubature formulas, we characterize them in two different ways: the first one by certain partitions of unity and the second one by a class of positive linear operators. Further, we show that there is a main difference between them and strongly positive definite cubature formulas. Indeed, we will show that the latter (strongly negative definite cubature formulas) can exist only if the domain of integration is a convex polytope. Finally, we will provide some numerical examples to

illustrate the efficiency of our cubature formulas.

In the fifth and last chapter, we have focused on the problem of approximating a definite integral of a given function f when, rather than its values at some points, a number of integrals of f over certain hyperplane sections of a d -dimensional hyper-rectangle C_d are only available. We develop several families of integration formulas, all of which are a weighted sum of integrals over some hyperplane sections of C_d , and which contain in a special case of our result multivariate analogues of the midpoint rule, the trapezoidal rule and Simpson's rule. Basic properties of these families are derived, in particular, we show that they satisfy a multivariate version of Hermite-Hadamard inequality. This latter does not require the classical convexity assumption, but it has weakened by a different kind of generalized convexity. As an immediate consequence of this inequality, we derive sharp and explicit error estimates for twice continuously differentiable functions. More precisely, we present explicit expressions of the best constants, which appear in the error estimates for the new multivariate versions of trapezoidal, midpoint, and Hammer's quadrature formulas. It is shown that, as in the univariate case, the constant of the error in the trapezoidal cubature formula is twice as large as that for the midpoint cubature formula, and the constant in the latter is also twice as large as for the new multivariate version of Hammer's quadrature formula. Numerical examples are given comparing these cubature formulas among themselves and with uniform and non-uniform centroidal Voronoi cubatures of the standard form, which use the values of the integrand at certain points. In fact, according to the data available to us in this problem, the motivation for this chapter is the following relevant question: how can we get a lower and upper estimate of the exact value of the integral of f over C_d ?

This problem arises in many applications, which mentioned above. The cubature formulas we have presented in this chapter have applications to the theory and practice of the numerical solution of PDEs using the so-called non conforming Crouzeix–Raviart element. In a forthcoming paper, see [1], we have used cubature formulas of this type for the approximate solution of a planar elasticity problem.

Contributions

The author has written two papers on the subject of the thesis. On the approximation of strongly convex functions by an upper or lower operator is published in Appl. Math. Comput. 247 (2014), 1129-1138. The article "New Cubature formulas and Hermite-Hadamard type inequalities using integrals over Some hyperplanes in the d -dimensional hyper-rectangle" accepted for publication in Appl Math Comput (2017) and has been the subject of chapter 5. Finally, The generalization given in Chapter 4 of the results on cubature formulas that approximate from above (or from below) the exact value of the integrals of every function having a certain type of convexity is new. A paper on this subject is in preparation.



Introduction générale

Motivation et objectifs de la thèse

Le but principal de cette thèse est de trouver une bonne approximation des fonctions de plusieurs variables par des opérateurs linéaires dont l'erreur d'approximation $A(f) - f$ garde un signe constant pour toute fonction f satisfaisant une certaine convexité généralisée. Nous nous concentrerons sur la classe des fonctions convexes et fortement convexes. L'approximation d'une fonction arbitraire f est, en général, très difficile à construire, mais nous savons parfois à l'avance que la fonction à approcher f satisfait certaines propriétés connues de structure et de régularité. Par exemple, on peut savoir que cette fonction vérifie un certain type de convexité, donc nous voudrions utiliser cette information afin d'obtenir une bonne approximation de f . Nous décrivons comment la connaissance a priori de cette information peut être utilisée pour déterminer une bonne majoration de l'erreur pour des fonctions continuellement différentiables avec des gradients Lipschitz continus. Plus précisément, nous montrons que les estimations d'erreur basées sur ces opérateurs sont toujours contrôlées par les constantes de Lipschitz des gradients, le paramètre de la convexité forte ainsi que l'erreur commise associée à l'utilisation de la fonction quadratique. En supposant en plus que la fonction que nous voulons approcher est également fortement convexe, nous établissons de meilleures bornes inférieures et supérieures pour les estimations d'erreur de l'approximation.

Les méthodes de quadrature multidimensionnelle jouent un rôle important, voire fondamental, en analyse numérique. Une analyse satisfaisante des erreurs provenant de l'utilisation des formules de quadrature multidimensionnelle est bien moins étudiée que dans le cas d'une variable. Nous proposons une méthode d'approximation de l'intégrale d'une fonction réelle donnée à plusieurs variables par des formules de quadrature, qui conduisent à des valeurs approchées par excès (respectivement par défaut) des intégrales des fonctions ayant un certain type de convexité. Nous verrons aussi, comme nous l'avons fait pour l'approximation des fonctions, que pour de telles formules d'intégration, on peut établir un résultat de car-

actérisation en termes d'estimations d'erreur. En outre, nous avons étudié le problème de l'approximation d'une intégrale définie d'une fonction donnée quand un certain nombre d'intégrales de cette fonction sur certaines sections hyperplanes d'un l'hyper-rectangle sont seulement disponibles.

La motivation derrière ce type de problème est multiple. Il se pose dans de nombreuses applications, en particulier en physique expérimentale et en ingénierie, où les valeurs standards des échantillons discrets des fonctions ne sont pas disponibles, mais où seulement leurs valeurs moyennes sont accessibles. Par exemple, ce type de données apparaît naturellement dans la tomographie par ordinateur avec ses nombreuses applications en médecine, radiologie, géologie, entre autres.

Plan de la thèse

Cette thèse se compose de cinq chapitres :

Nous poursuivrons, d'abord, l'introduction des travaux antérieurs concernant ce sujet, et présentons aussi un résumé des résultats que nous avons obtenus.

Le premier chapitre introduit la convexité habituelle et ses généralisations. Il comprend presque tout ce qui est essentiel concernant les résultats de caractérisation des fonctions convexes (éventuellement régulières). Il fournit aussi un ensemble de preuves étonnamment courtes utilisant des caractérisations bien connues de convexité pour des fonctions à une seule variable. Certains résultats de ce domaine sont peu connus : nous avons donc essayé d'en offrir une vision synthétique et unifiée. Une des propriétés la plus importante d'une fonction convexe est que la fonction contrôle toujours son approximation de Taylor du premier ordre (linéaire). Malheureusement, en général, il est encore difficile de borner l'erreur introduite par une telle approximation si aucune information supplémentaire n'est disponible. Par conséquent, nous devons étendre la notion de convexité classique. Nous avons réalisé que la condition naturelle que nous pouvons imposer à la fonction est d'appartenir à la classe des fonctions fortement convexes. De plus, nous établirons une relation étroite entre la convexité classique et la convexité forte qui nous a aidé à établir quelques caractérisations importantes pour ce type de fonctions. Il est également montré que, sous des restrictions du type convexité forte, nous pouvons obtenir de meilleures bornes inférieures et supérieures pour l'erreur dans l'approximation linéaire que celles qui sont obtenues pour la convexité classique. C'est l'un des principaux objectifs de ce chapitre. Pour cette fin, nous considérons le cas où, en outre, les gradients sont Lipschitz continus. Dans ce contexte, nous présentons quelques théorèmes de caractérisation et donnons également des bornes d'erreur, qui sont contrôlées et améliorées

par rapport à celles obtenues pour la convexité ordinaire. Enfin, nous essayons de fournir plus de détails dans les preuves là où il nous semblait nécessaire de le faire (en se basant sur les travaux [1, 7, 8, 10]).

Dans le deuxième chapitre, en raison du besoin urgent de quelques concepts et théorèmes de caractérisation pour cette étude, nous commençons par donner deux définitions équivalentes d'un prototype et ensuite nous énonçons quelques théorèmes fondamentaux bien connus et les propriétés d'un tel objet géométrique. Par la suite, nous définissons la notion de coordonnées barycentriques généralisées par rapport à un ensemble arbitraire de points dans $\mathbf{R}^d$, ou équivalent, par rapport à un polytope (convexe). Nous montrons alors que ces coordonnées existent toujours pour tout ensemble fini de points donnés. Ce résultat d'existence est dû à Kalman dans les années soixante [26, Théorème 2]. De plus, ce chapitre introduit les triangulations de Delaunay comme géométriquement duales aux diagrammes de Voronoi. Nous résumons les propriétés fondamentales de telles triangulations largement utilisées. Sous l'hypothèse de convexité, nous fournissons également une méthode d'approximation que nous appelons approximation barycentrique. Cette classe d'opérateurs (linéaires) satisfait la condition de croissance pour toute fonction convexe. Enfin, nous donnons un résultat de caractérisation pour ces opérateurs en terme de leurs estimations d'erreur. Un tel théorème de caractérisation est dû à Guessab dans son récent article [2].

Dans le troisième chapitre, nous avons proposé une méthode convenable et pratique pour approcher une fonction réelle à plusieurs variables par des opérateurs linéaires vérifiant la condition de décroissance pour toute fonction fortement convexe. Nous avons utilisé ce résultat pour établir une meilleure estimation de l'erreur pour des fonctions continuellement différentiables avec des gradients de Lipschitz continus. Plus précisément, nous montrons que les estimations d'erreur basées sur ces opérateurs sont toujours contrôlées par les constantes de Lipschitz des gradients, le paramètre de convexité de la convexité forte et l'erreur associée à l'utilisation de la fonction quadratique, comme on le verra dans les théorèmes 3.2.1 et 3.2.3. En supposant en plus que la fonction que nous voulons approcher est fortement convexe, nous fournissons des bornes supérieures ainsi que des bornes raffinées inférieures pour les estimations d'erreur, voir les Corollaires 3.2.2 et 3.2.4. Comme application, nous définissons et étudions une classe d'opérateurs linéaires sur un polytope arbitraire vérifiant la condition de décroissance et qui approchent les fonctions fortement convexes. Enfin, nous présentons un exemple numérique illustrant la méthode proposée. Ainsi, l'une des principales raisons qui a retenu toute notre attention sur une telle classe de fonctions est que ces dernières sont largement utilisées dans la théorie économique (voir [1]), et sont également essentielles à la théorie de l'optimisation (voir [2]). En effet, dans le cadre de la minimisation des fonctions, cette notion de convexité a des implications importantes et bien connues.

Dans le chapitre 4, nous avons développé certains résultats des travaux [1, 2, 3, 4] en introduisant une nouvelle classe de quadrature multidimensionnelle, qui conduisent à des valeurs

approchées par excès (respectivement par défaut) la valeur exacte des intégrales de toute fonction ayant un certain type de convexité. Tout d'abord, nous aimerions mentionner que tous ces résultats ont été déjà établis dans le contexte de la notion classique de convexité. Ici, notre objectif est d'étendre les idées qui y sont données sous certains types de convexité généralisée. Dans ce chapitre, nous présentons d'abord quelques définitions et notations puis, deux résultats de caractérisation de toute fonctionnelle linéaire $C^{1,1}(\cdot) \rightarrow \mathbf{R}$, qui est positive sur l'ensemble des fonctions convexes. De plus, nous définissons deux nouvelles classes de formules de quadrature, que nous appelons les formules de quadrature définies fortement positives, respectivement négatives. Nous appliquons ensuite nos résultats généraux au cas où la fonctionnelle est l'erreur fonctionnelle de nos formules de quadrature. Plus précisément, nous montrons que pour les fonctions appartenant à $C^{1,1}(\cdot)$, les estimations d'erreur basées sur ces formules de quadrature sont toujours contrôlées par les constantes de Lipschitz des gradients, les différents types de convexité et l'erreur associée à l'utilisation de la fonction quadratique. De plus, en sachant que si la fonction à intégrer satisfait la convexité classique ou la convexité forte, nous établissons de bonnes bornes supérieures ainsi que des bornes inférieures raffinées pour les estimations d'erreur. L'un des résultats intéressants de ce chapitre est que pour des formules de quadrature définies fortement positives, nous établissons des résultats de caractérisation en terme de la partition de l'unité du domaine d'intégration. Nous montrons également comment les construire en utilisant la méthode de décomposition du domaine d'intégration. Le même résultat a été établi pour les formules de quadrature définies fortement négatives. Nous les caractérisons de deux manières différentes : la première par certaines partitions d'unité et la seconde par une classe d'opérateurs linéaires positifs. De plus, nous montrons qu'il existe une différence principale entre celles-ci et les formules de quadrature définies fortement positives. En effet, nous montrerons que ces dernières (formules de quadrature définies fortement négatives) ne peuvent exister que si le domaine d'intégration est un polytope convexe. Enfin, nous fournirons quelques exemples numériques pour illustrer l'efficacité de nos formules de quadrature.

Dans le cinquième et dernier chapitre, nous nous sommes concentrés sur le problème de l'approximation d'une intégrale définie d'une fonction donnée f quand, au lieu de ses valeurs en des points définis, un certain nombre d'intégrales de f sur des sections hyperplanes d'un hyper-rectangle C_d sont seulement disponibles. Nous développons plusieurs familles de formules d'intégration, qui sont toutes une somme pondérée d'intégrales sur certaines sections hyperplanes de C_d . Ces formules de quadrature sont des versions multidimensionnelles naturelles des formules du point milieu, des trapèzes et de Simpson. Des propriétés fondamentales de ces formules de quadrature sont établies, plus particulièrement nous montrons qu'elles vérifient une version multidimensionnelle de l'inégalité Hermite-Hadamard. Cette dernière n'exige pas l'hypothèse de convexité classique, mais il nécessite un autre type de convexité généralisée. Comme conséquence immédiate de cette inégalité, nous déterminons des estimations d'erreur explicites pour les fonctions continuellement différentiables. Plus précisément, nous présentons des expressions explicites de meilleures constantes qui ap-

paraissent dans les estimations d'erreur pour les nouvelles formules de quadrature. Nous montrons que, comme dans le cas univarié, la constante de l'erreur dans la formule de quadrature multidimensionnelle des trapèzes est deux fois plus grande que celle de la formule de quadrature multidimensionnelle du point milieu, et que la constante dans cette dernière est aussi deux fois plus grande que pour la nouvelle version multidimensionnelle de la formule de quadrature de Hammer.

Des exemples numériques sont donnés en comparant ces formules de quadrature entre elles et avec des formules de quadrature de Voronoï centrales et non uniformes de la forme standard qui utilisent les valeurs de la fonction à intégrer en certains points. Les formules de quadrature que nous avons présentées dans ce chapitre trouvent leur intérêt pour la résolution numérique des équations aux dérivées partielles en utilisant l'élément de Crouzeix-Raviart dit non conforme. Dans la publication [1], les formules de quadrature de ce type ont été utilisées pour la résolution numérique d'un problème d'élasticité linéaire.

Enfin, nous présentons et discutons deux perspectives liées à notre travail concernant l'extension de ces résultats à d'autre type de convexité généralisée, par exemple, la convexité uniforme. Nous envisageons par la suite d'étendre les formules de quadrature multidimensionnelle au cas où certaines intégrales sont connues sur chaque facette d'une triangulation simpliciale

Contributions de la thèse

L'auteur a rédigé trois articles dans le cadre du sujet de la thèse :

1- L'article " On the approximation of strongly convex functions by an upper or lower operator" est publiée dans Appl. Math. Comput. 247 (2014), 1129-1138." constitue le cœur de la thèse et fait l'objet du chapitre 3.

2- L'article "New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle" accepté pour publication dans Appl. Math. Comput. (2017) et a fait l'objet du chapitre 5.

3- Enfin, la généralisation donnée au chapitre 4 des résultats sur les formules de quadrature multidimensionnelle, qui conduisent à des valeurs approchées par excès (respectivement par défaut) de la valeur exacte de l'intégrale de toute fonction ayant un certain type de convexité fait l'objet d'une publication en cours de révision.

1 Convex Functions and their Generalizations

The purpose of this chapter is to introduce the reader to usual convexity and its generalizations. Section 1.1, which is mainly for reference, collects in particular the most relevant and essential characterization results for (possibly smooth) convex functions. The presentation is essentially based on [1, 7, 8, 10], trying to provide more details in the proofs where it felt needed. However, our approach provides a unifying framework with often surprisingly short proofs using well-known characterizations of convexity for functions of one variable. One of the most important properties of the usual convexity is that the function always dominates its first order (linear) Taylor approximation. Unfortunately, in general, it is still difficult to get better bounds on the error introduced by such an approximation if we have no additional information.

For this reason, we need to relax the notion of classical convexity. It turns out, as will be clarified by the analysis below, that the natural condition that we can impose on the function is to belong the class of strongly convex functions. After providing an intimate relationship between convexity and strong convexity, we establish some characterizations of these kind of functions. It is also showing that in this setting, we can obtain better lower and upper bounds in linear approximation than that from usual convexity. This is the aim of section 1.2.

In order to obtain better bounds for the linear approximation, under (possibly strong convexity) convexity assumption, Section 1.3 considers the case when, in addition, the gradients are Lipschitz continuous. In this case, we provide some characterization theorems and also give more controlled and improved error bounds than those obtained for ordinary convexity.

1.1 Usual convexity

1.1.1 Notation and Terminology

More special notions are introduced gradually throughout this document. We use the standard notation $\mathbf{R}$ for the set of real numbers, and we let

$$\begin{aligned}\mathbf{R}^{\geq 0} &\triangleq \{x \in \mathbf{R} \mid x \geq 0\}, \\ \mathbf{R}^+ &\triangleq \{x \in \mathbf{R} \mid x > 0\}, \\ \mathbf{R}^{\geq 0}_d &\triangleq \{x \in \mathbf{R}^d \mid x_i \geq 0\}.\end{aligned}$$

In other words, $\mathbf{R}^{\geq 0}$ consists of all nonnegative real numbers, and $\mathbf{R}^+$ denotes the set of all positive real numbers. Throughout, $\mathbf{R}^d$ denotes the d -dimensional Euclidean space. We may refer to its elements interchangeably as vectors or points. For a point $\mathbf{x} \in (x_1, x_2, \dots, x_d) \in \mathbf{R}^d$,

$$\|\mathbf{x}\|_2 \triangleq \sqrt{x_1^2 + x_2^2 + \dots + x_d^2}$$

is the Euclidean norm (also called the length) of $\mathbf{x}$, and for $\mathbf{x}, \mathbf{y} \in \mathbf{R}^d$, $\mathbf{x} \cdot \mathbf{y} \triangleq x_1 y_1 + x_2 y_2 + \dots + x_d y_d$ is the usual scalar product on $\mathbf{R}^d$. Vectors in $\mathbf{R}^d$ will interchangeably be identified with column matrices. Thus, to us

$$(x_1, x_2, \dots, x_d) \quad \text{and} \quad \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$$

denote the same object. For $\mathbf{x}, \mathbf{y} \in \mathbf{R}^d$, the notation $[\mathbf{x}, \mathbf{y}]$ is often used to denote the line segment between $\mathbf{x}$ and $\mathbf{y}$, that is,

$$[\mathbf{x}, \mathbf{y}] \triangleq \{\mathbf{z} \in \mathbf{R}^d \mid \mathbf{z} = (1 - \lambda)\mathbf{x} + \lambda\mathbf{y}, 0 \leq \lambda \leq 1\}.$$

1.1.2 Convex functions of one variable

We start by recalling some well known general criteria for convexity of real-valued convex functions of one variable, which we shall use later. A real-valued function f defined on an interval $I \subseteq \mathbf{R}$ is convex if the inequality

$$f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y)$$

holds for every $x, y \in I$ and every $0 \leq \lambda \leq 1$. The following properties characterize the convexity of a function of one variable by means of its first and second derivatives, see [9, Theorem 1.6, Corollary 1.1, Theorem 1.8]. This theorem may serve as a basis for the corresponding characterizations in the multidimensional case.

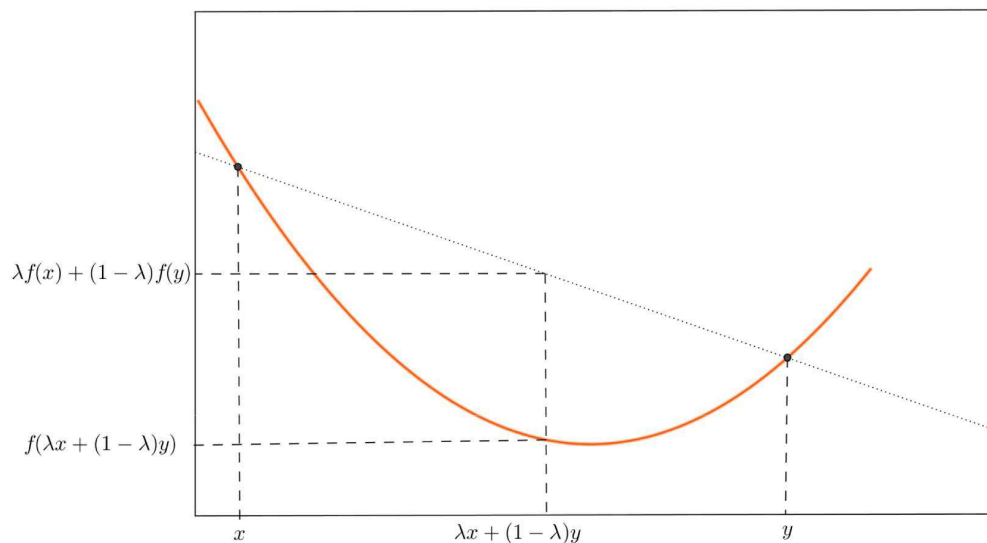


Figure 1.1 – illustration of the inequality $f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y)$.

Theorem 1.1.1 (Convexity criteria) Let $f : I \rightarrow \mathbb{R}$ be a continuous function defined on an open interval $I \subset \mathbb{R}$.

1. If f is differentiable, then f is convex if and only if it lies above or on all of its tangents. In other words $f(y) \geq f(x) + f'(x)(y - x)$ for all x and y in I .
2. If f is differentiable, then f is convex if and only if f' is increasing.
3. If f is two times differentiable, then f is convex if and only if $f'' \geq 0$ (i.e., $f''(x) \geq 0$ for all $x \in I$).

We now present a result for extrema of a function commonly known as one of Fermat's theorems. This classical result may be found in [3, Theorem 1.3.7].

Theorem 1.1.2 (Fermat's theorem on extrema) Let $f : I \rightarrow \mathbb{R}$ be a differentiable function defined on an open interval $I \subset \mathbb{R}$. If $x \in I$ is a local extremum, then $f'(x) = 0$.

1.1.3 Convex sets

We start with the definition of a convex set and its characterization. We also give some operations, which preserve convexity of sets.

Convex Functions and their Generalizations

Definition 1.1.3 (Convex set) A subset C of $\mathbf{R}^d$ is called convex if the line segment between any two points in C lies in C , i.e.,

$$(1 - \lambda)x + \lambda y \in C,$$

holds for all $x, y \in C$ and $\lambda \in [0, 1]$.

The above definition can be generalized from two points to any number of points k . A convex combination of points $x_1, x_2, \dots, x_k \in C$ is any point of form $\lambda_1 x_1 + \lambda_2 x_2 + \dots + \lambda_k x_k$, where $\lambda_i \geq 0, i \in 1, \dots, k$ and $\lambda_1 + \lambda_2 + \dots + \lambda_k = 1$.

We have the following simple characterization of convex sets, see, e. g., [10, Theorem 2.2], which can be shown by induction.

Theorem 1.1.4 (Characterization of convex sets) A set C in $\mathbf{R}^d$ is convex if and only if it is closed with respect to taking all convex combinations of its elements, i.e., if and only if any convex combination of vectors from C again is a vector from C .

The following result outlines properties of convex sets, see, e. g., [2, 10].

Theorem 1.1.5 (Convexity-preserving operations of convex sets) The convexity property of a set is also preserved by many operations: namely, the operations of taking:

1. Intersection.
2. Scalar multiplication.
3. Closure.
4. Interior.
5. Coordinate Projection.
6. Translate of a set.
7. Sum of set.

Next we consider the notion of extreme points.

Definition 1.1.6 Let $C \subseteq \mathbf{R}^d$ be a convex set. A point $x \in C$ is called an extreme point of C if $x \notin t y + (1 - t) z$ for $y, z \in C$ and $t \in (0, 1)$ implies $x \notin y \cup z$.

Compact convex sets can be described via their extreme points as stated in the next result, see, e. g., [1, Theorem 6.35].

Theorem 1.1.7 (Krein-Milman theorem) Let $C \subset \mathbb{R}^d$ be a compact convex set. Then the set of extreme points of C is not empty. Furthermore, every $x \in C$ may be expressed as a convex combination of finitely many extreme points of C .

1.1.4 Multivariate convex functions

The following is the traditional definition of a convex function, which is sometimes referred to as zero-order condition.

Definition 1.1.8 (The zero order condition) A real-valued function $f : C \rightarrow \mathbb{R}$ defined on a convex subset C of $\mathbb{R}^d$ is said to be convex on C if

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda)f(y) \quad (1.1)$$

for all $x, y \in C$ and $0 \leq \lambda \leq 1$.

If f is a convex function on C , then f is said to be a concave function.

- Function is below a linear interpolation from x to y .
- Implies that all local minima are global minima.

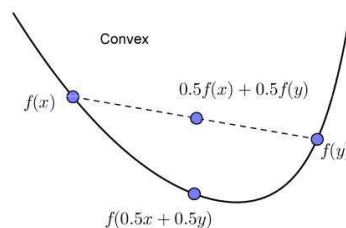


Figure 1.2 – Any minimum of convex function is a global minimum.

If $f(\lambda x + (1-\lambda)y) < \lambda f(x) + (1-\lambda)f(y)$ for all $x, y \in C$, $x \neq y$ and $0 < \lambda < 1$, then we say that f is strictly convex. The strict convexity implies at most one global minimum.

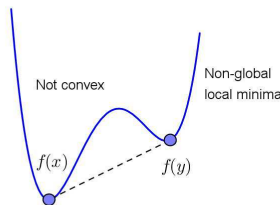


Figure 1.3 – non-global local minimal.

Remark 1.1.9 In connection with the last definition, we can note the following equivalent geometric meaning of the definition, if x and y are two distinct points belonging to the domain C of function f , and consider the point $\lambda x + (1 - \lambda)y$ with $\lambda \in [0, 1]$. The function f is convex on the domain C iff for every x and y belong to the domain C of f , the line segment (chord) connecting the point $x, f(x)$ to $y, f(y)$ is always above or on the curve f . Or equivalently, the value of f at points $\lambda x + (1 - \lambda)y$ on the line segment $\lambda x + (1 - \lambda)y$ is less than or equal to the height of the chord which connects the points $x, f(x)$ and $y, f(y)$. Analogously, f is concave iff the line segment (chord) lies below or on the curve f . This geometric meaning illustrated in the figures below 1.4, 1.6, 1.8 and 1.10.

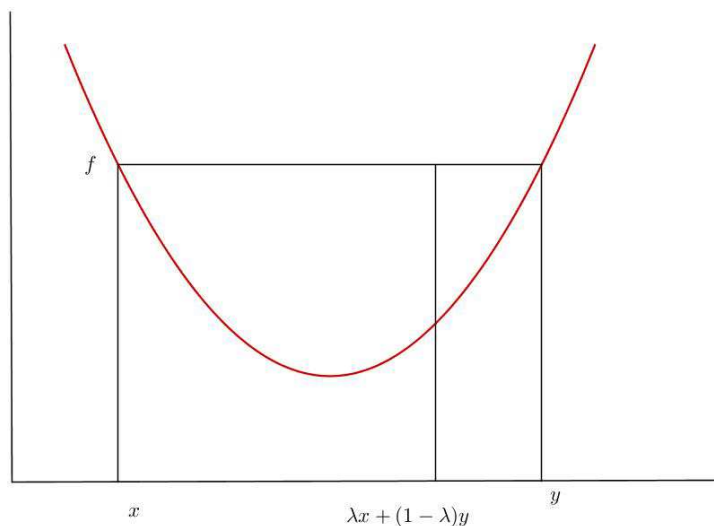
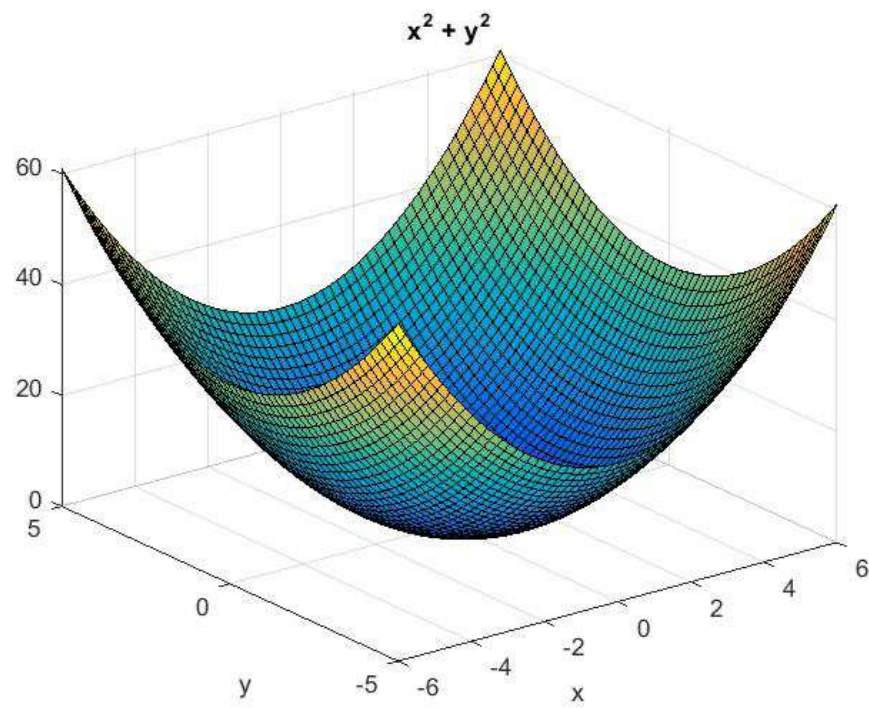
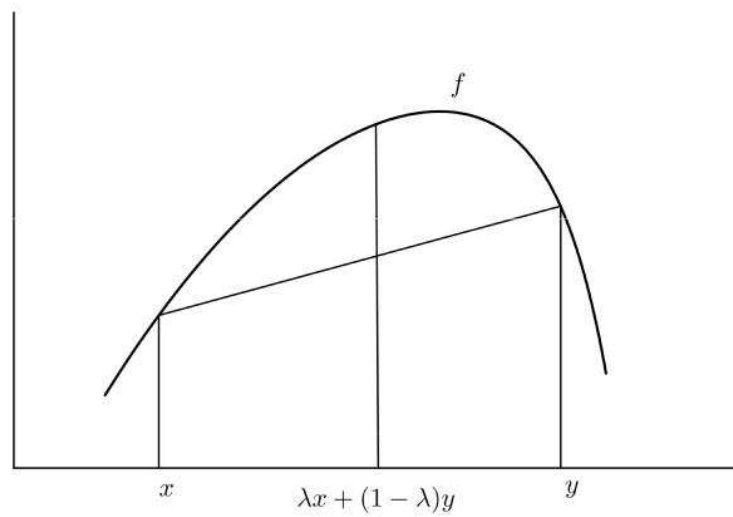


Figure 1.4 – convex function.

Figure 1.5 – **convex function**.Figure 1.6 – **concave function**.

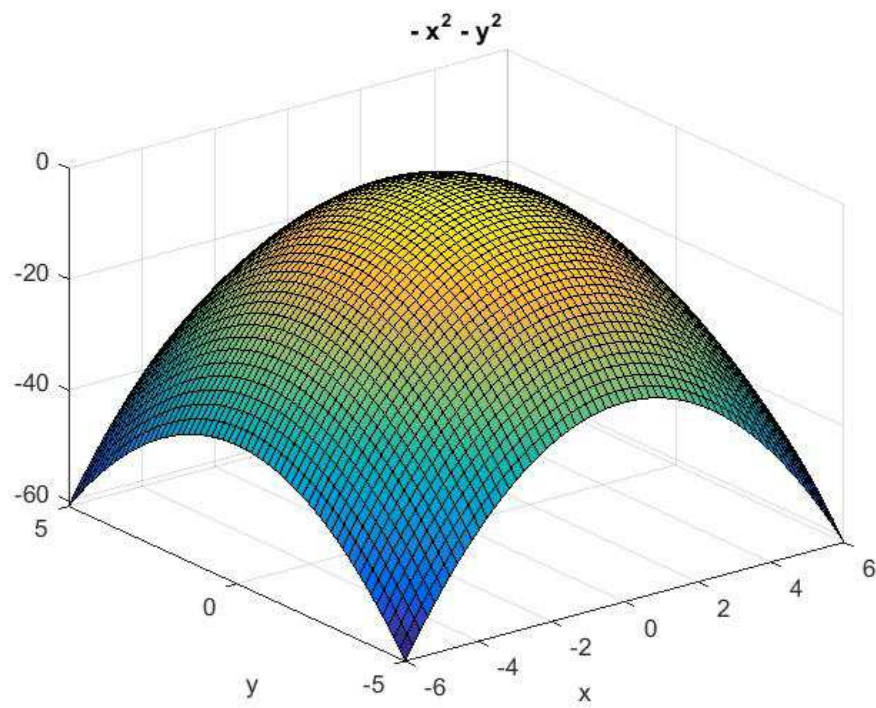


Figure 1.7 – **concave function.**

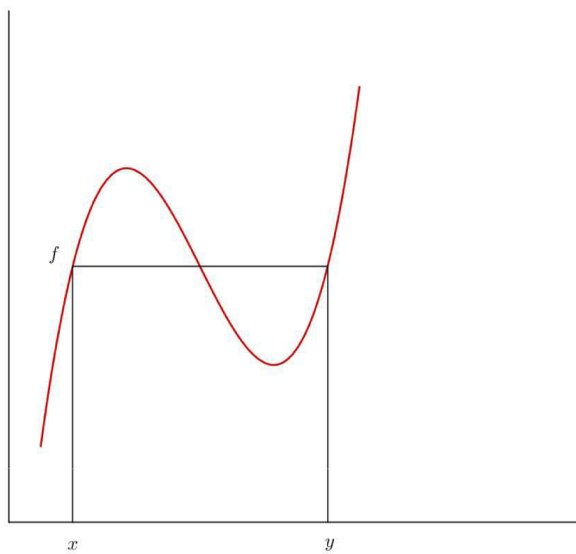


Figure 1.8 – **neither convex nor concave.**

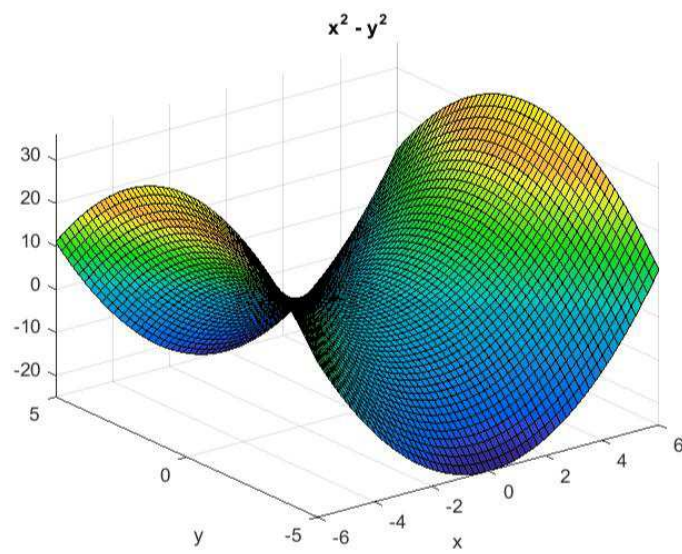


Figure 1.9 – **neither convex nor concave.**

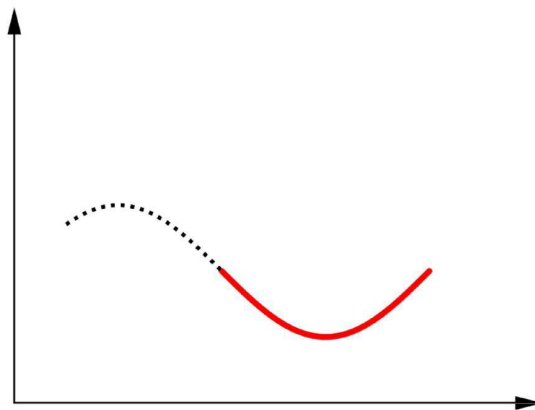


Figure 1.10 – **convex and concave.**

Convex Functions and their Generalizations

The function in Fig.1.4 is convex, Fig.1.6 is concave and Fig.1.8 is neither. The function in Fig.1.10 is convex on the part where it is solid and concave on the part where it is dotted.

The following result outlines some properties of convex functions, and it also gives some ways to construct new convex functions from given convex functions, for more details see [8, Section 3.2].

Theorem 1.1.10 (Convexity-preserving operations of convex functions) *The convexity property of a function is also preserved by many operations: namely, the operations of taking:*

1. *Nonnegative weighted sum.*
2. *composition with affine function.*
3. *Pointwise maximum and supremum.*
4. *Composition.*
5. *minimization.*
6. *Perspective.*

By induction on the number of points, convexity can also be characterized using general convex combinations of more than two points. This is the so-called Jensen's inequality. An elementary proof may be found in [1, Theorem 7.5].

Theorem 1.1.11 (Jensen's inequality) *Let $C \subseteq \mathbb{R}^d$ be a convex set, and let $f : C \rightarrow \mathbb{R}$ be convex on C . If $\lambda_1, \lambda_2, \dots, \lambda_k \in [0, 1]$, $\sum_{i=1}^k \lambda_i = 1$, and $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k \in C$, then*

$$f\left(\sum_{i=1}^k \lambda_i \mathbf{x}_i\right) \leq \sum_{i=1}^k \lambda_i f(\mathbf{x}_i).$$

Continuity is an important property of a convex function. The following theorem shows that a convex function is automatically continuous on an open convex set or the interior of its domain, see [5, Theorem 1.3.12].

Theorem 1.1.12 (Continuity property of convex functions) *Let $C \subseteq \mathbb{R}^d$ be an open convex set. Let $f : C \rightarrow \mathbb{R}$ be convex. Then f is continuous on C .*

For a continuously differentiable function f defined on an open convex set $C \subseteq \mathbb{R}^d$, we denote its gradient at $\mathbf{x} \in C$, by

$$\nabla f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}), \frac{\partial f}{\partial x_2}(\mathbf{x}), \dots, \frac{\partial f}{\partial x_d}(\mathbf{x}) \end{pmatrix}.$$

Convex functions have a nice property that a local minimum of the function in the convex set is namely automatically a global minimum. This is the reason why convex functions are important in optimization problems as well as in other areas of mathematics.

Theorem 1.1.13 (Global minimum) Let $f : C \rightarrow \mathbb{R}$ be a differentiable convex function defined on an open convex set $C \subset \mathbb{R}^d$. Let $\mathbf{x}^* \in C$. Then the following three statements are equivalent.

- (i) $\mathbf{x}^*$ is a local minimum for f .
- (ii) $\mathbf{x}^*$ is a global minimum for f .
- (iii) $\nabla f(\mathbf{x}^*) = \mathbf{0}$, (i.e., all partial derivatives $\frac{\partial f}{\partial x_i}$ at $\mathbf{x}^*$ are zero).

Proof The direction (ii) implies (i) is trivial. We now prove that (i) implies (iii). Assume that $\mathbf{x}^*$ is a local minimum. Let $i \in \{1, 2, \dots, d\}$ and consider the one (real) variable function $g(t) = f(\mathbf{x}^* + t\mathbf{e}_i)$, where $\mathbf{e}_i$ denotes the i th unit vector of $\mathbb{R}^d$: its i th component is one, and all others zero. Note that since C is an open set, $\mathbf{x}^* + t\mathbf{e}_i \in C$ for sufficiently small $t \in \mathbb{R}$. Furthermore g is differentiable at $t = 0$ and that

$$g'(0) = \frac{\partial f}{\partial x_i}(\mathbf{x}^*). \quad (1.2)$$

Since $\mathbf{x}^*$ is a local minimum point of f , we deduce that $t = 0$ is a local minimum of g , then according to Fermat's theorem, see Theorem 1.1.2, 0 should be a critical point so $g'(0) = 0$. Hence by (1.2) we conclude that $\frac{\partial f}{\partial x_i}(\mathbf{x}^*) = 0$. Since this holds for any $i \in \{1, 2, \dots, d\}$ assertion (iii) follows. Note that we have proven that the implications holds for any differentiable function, which need not be convex.

It remains to show that (iii) implies (ii). Let $\mathbf{x}^* \in C$ be a stationary point, i.e., $\nabla f(\mathbf{x}^*) = \mathbf{0}$. Assume, on the contrary, that $\mathbf{x}^*$ is not a global minimum, then there exists $\mathbf{x} \in C$ such that $f(\mathbf{x}) < f(\mathbf{x}^*)$. Let us consider the one variable function $g : [0, 1] \rightarrow \mathbb{R}$, defined by $g(t) = f(t\mathbf{x} + (1-t)\mathbf{x}^*)$. Note that g is convex and differentiable on $[0, 1]$, and moreover there holds

$$g'(0) = \nabla f(\mathbf{x}^*) \cdot (\mathbf{x} - \mathbf{x}^*) \leq 0.$$

Therefore, using convexity of g , we obtain

$$\begin{aligned}
 0 &\in g''(0) \\
 &\in \lim_{t \rightarrow 0^+} \frac{g(t) - g(0)}{t} \\
 &\in \lim_{t \rightarrow 0^+} \frac{g(t) - (1-t)g(0) - tg(1)}{t} \\
 &= \lim_{t \rightarrow 0^+} \frac{tg(1) - (1-t)g(0) - tg(0)}{t} \\
 &\in g(1) - g(0) \\
 &\in f(\mathbf{x}) - f(\mathbf{x}^*) < 0.
 \end{aligned}$$

Thus, we have arrived at a contradiction. Hence, $\mathbf{x}^*$ must be a global minimum. ■

The role of convexity in linking the global maximum and extreme points in optimization theory is illustrated by the so-called maximum principle.

Theorem 1.1.14 (The maximum principle) Let $C \subseteq \mathbb{R}^d$ be a compact convex set and let $f: C \rightarrow \mathbb{R}$ be a continuous convex function. Then f attains its maximum at an extreme point of C .

Proof Since C is compact and f is continuous then by Weierstrass's Theorem, there exists $\bar{\mathbf{x}} \in C$ with $f(\bar{\mathbf{x}}) \in \max_{\mathbf{x} \in C} f(\mathbf{x})$. By Theorem 1.1.7, the set C is the convex hull of its extreme points, so we can write

$$\bar{\mathbf{x}} \in \sum_{i=1}^N t_i \mathbf{v}_i$$

for each $i, i \in \{1, 2, \dots, N\}$, $t_i \geq 0$, $\sum_{i=1}^N t_i = 1$, and extreme points $\mathbf{v}_1, \dots, \mathbf{v}_N$ of C . Since

$$f(\mathbf{v}_i) \leq f(\bar{\mathbf{x}}), \quad (1.3)$$

we get by convexity of f

$$f(\bar{\mathbf{x}}) \leq f\left(\sum_{i=1}^N t_i \mathbf{v}_i\right) \leq \sum_{i=1}^N t_i f(\mathbf{v}_i) \leq f(\bar{\mathbf{x}}).$$

Thus, we arrive at the equality

$$\sum_{i=1}^N t_i (f(\bar{\mathbf{x}}) - f(\mathbf{v}_i)) = 0.$$

But from (1.3), we know that the above is a sum of nonnegative terms summing to zero. It implies that each term in the above sum is zero, and hence $f(\bar{\mathbf{x}}) = f(\mathbf{v}_i)$ for some i . Therefore, the maximum of f is attained at an extreme point of C . ■

1.1.5 Characterizations of convexity

There are multiple ways to characterize a convex function, each of which may be convenient or insightful in different contexts. Below we present only the most commonly used ones.

Given a function $f : C \rightarrow \mathbb{R}$ defined on a convex set C . The definition of the convex function is intimately related to the concept of a convex set. The graph of a function f is defined as,

$$\text{Graph}(f) = \{(x, f(x)) \mid x \in C\} \subset \mathbb{R}^d \times \mathbb{R}.$$

The epigraph of f is defined as the set of points $(x, t) \in C \times \mathbb{R}$ lying on or above the graph of the function:

$$\text{epi}(f) = \{(x, t) \in C \times \mathbb{R} : f(x) \leq t\}.$$

The following theorem indicates the relation between convex function and convexity of its epigraph. We refer to [4, Proposition 2.6] for an elementary proof.

Theorem 1.1.15 (Characterization in terms of graphs) *The function f is convex iff the set $\text{epi}(f)$ is convex.*

This property is useful because it allows us to check convexity of a multivariate function by checking convexity of functions of one variable, for which there exist many simpler criteria.

Theorem 1.1.16 (One-variable characterization) *Let $f : C \rightarrow \mathbb{R}$ be a real-valued function defined on an open convex set $C \subset \mathbb{R}^d$. For each $x \in C$ and $z \in \mathbb{R}^d$, we define the interval $I \subseteq \mathbb{R}$ as $I = \{t \in \mathbb{R} : x + t(z-x) \in C\}$ and the function $g : I \rightarrow \mathbb{R}$ given by $g(t) = f(x + t(z-x))$. Then f is convex if and only if each such function g (for all $x \in C, z \in \mathbb{R}^d$) is convex.*

As a special case of Theorem 1.1.16, we obtain the following result.

Corollary 1.1.17 *Let $f : C \rightarrow \mathbb{R}$ be a real-valued function defined on an open convex set $C \subset \mathbb{R}^d$. Then the function f is convex on C if and only if the function $g : [0, 1] \rightarrow \mathbb{R}$ given by $g(t) = f((1-t)x + ty)$ is convex (as a univariate function) for all $x \in C$ and all $y \in C$.*

When f is smooth enough (in some sense convex with some continuity property of the derivatives), as for univariate functions, we can give other characterizations of convexity. If a function is differentiable then, as for univariate functions, we can give characterizations of convex functions using derivatives, which essentially states that the tangent hyperplanes of convex functions are always underestimates the function.

The following theorem gives the first order characterization of convex functions.

Convex Functions and their Generalizations

Theorem 1.1.18 (The first-order condition for convexity: Gradient inequality) Let $C \subseteq \mathbb{R}^d$ be a nonempty open convex set and let $f: C \rightarrow \mathbb{R}$ be a continuously differentiable function.

Then f is convex if and only if for any $\mathbf{x}, \mathbf{y} \in C$ we have

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (\mathbf{y} - \mathbf{x}). \quad (1.4)$$

Proof We first assume that f is convex. Let us fix $\mathbf{x} \in C$ and consider the function

$$g(\mathbf{y}) = f(\mathbf{y}) - \nabla f(\mathbf{x}) \cdot (\mathbf{y} - \mathbf{x}), \quad \mathbf{y} \in C.$$

Since $h(\cdot) = \nabla f(\mathbf{x}) \cdot (\cdot - \mathbf{x})$ is an affine function, therefore $h(\cdot)$ is a convex function, and the sum of two convex functions is a convex function, then g is a convex function on C . Furthermore, we observe that

$$\nabla g(\mathbf{x}) = \nabla f(\mathbf{x}) - \nabla f(\mathbf{x}) = \mathbf{0},$$

then $\mathbf{x}$ is a critical point of g . Applying Theorem 1.1.13, we have for all $\mathbf{y} \in C$

$$g(\mathbf{x}) \leq g(\mathbf{y}),$$

which is equivalent to the desired inequality (1.4).

To prove the converse, assume that the gradient inequality (1.4) holds. By the one-variable characterization of convexity, see Theorem 1.1.16, all we should prove is the convexity of every one-dimensional function

$$g(t) = f(\mathbf{x} + t\mathbf{z})$$

for all fixed $\mathbf{x} \in C$, $\mathbf{z} \in \mathbb{R}^d$, such that $\mathbf{x} + t\mathbf{z} \in C$. Let us define $I = \{t \in \mathbb{R} : \mathbf{x} + t\mathbf{z} \in C\}$. Since C is an open convex set and $\mathbf{x} \in C$, then clearly I is a non-empty open interval containing zero. Moreover, by (1.4), we have for all $t, t^0 \in I$,

$$\begin{aligned} f(\mathbf{x} + t\mathbf{z}) &\geq f(\mathbf{x} + t^0\mathbf{z}) + \nabla f(\mathbf{x} + t^0\mathbf{z}) \cdot (\mathbf{x} + t\mathbf{z} - (\mathbf{x} + t^0\mathbf{z})) \\ &= f(\mathbf{x} + t^0\mathbf{z}) + \nabla f(\mathbf{x} + t^0\mathbf{z}) \cdot (t - t^0)\mathbf{z} \\ &= f(\mathbf{x} + t^0\mathbf{z}) + (t - t^0) \nabla f(\mathbf{x} + t^0\mathbf{z}) \cdot \mathbf{z}, \end{aligned}$$

which is equivalent to

$$g(t) \geq g(t^0) + g'(t^0)(t - t^0).$$

Hence by Theorem 1.1.1, this implies that g is convex. ■

Theorem 1.1.18 means that the linear Taylor approximation is a lower estimate, i.e, the tangent of convex function always lies under the function at any point, such a tangent is called a supporting hyperplane of the convex function. Another type of a first order characterization of convexity is the monotonicity property of the gradient. In the one-dimensional case, this

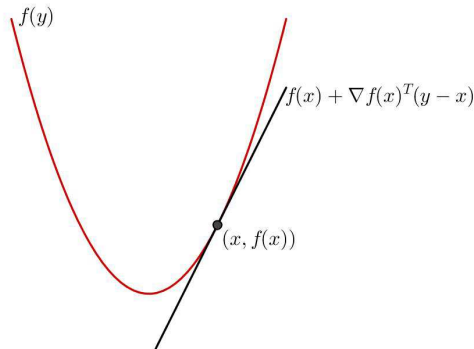


Figure 1.11 – If f is convex and differentiable, then $f(x) \leq \nabla f(x)^T(y - x) + f(x)$ for all x, y belonging to domain of f (the first order characteristic of a convex function).

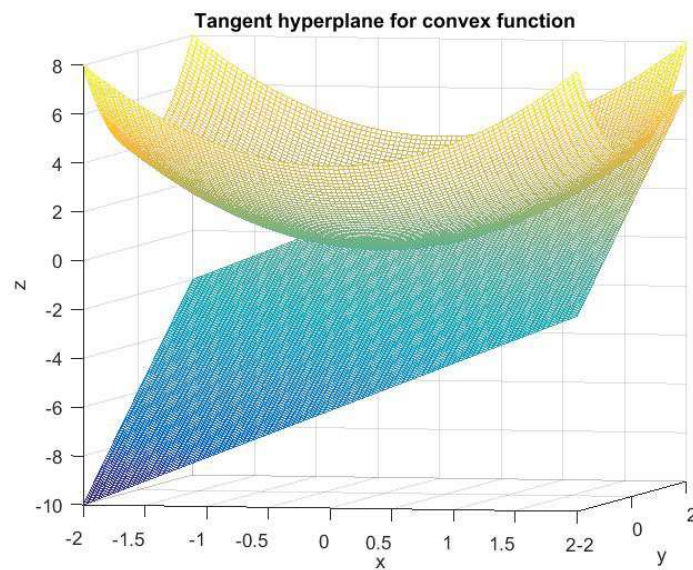


Figure 1.12 – If f is convex and differentiable, then $f(x) \leq \nabla f(x)^T(y - x) + f(x)$ for all x, y belonging to domain of f (the first order characteristic of a convex function).

means that the derivative is nondecreasing, but another definition of monotonicity is required in the multivariate setting.

Definition 1.1.19 A mapping $F : D \subseteq \mathbb{R}^d \rightarrow \mathbb{R}^d$ is monotone on D if

$$\langle F(x) - F(y), x - y \rangle \geq 0, \quad \forall x, y \in D. \quad (1.5)$$

Convex Functions and their Generalizations

If we let $F \in \mathcal{R}^d$ in the above definition, then it follows the following theorem which states that, for convex function f , its gradient ∇f is a monotone mapping.

Theorem 1.1.20 (Characterization via the monotonicity of the gradient) Let $C \subseteq \mathbb{R}^d$ be a non empty open convex set and let $f: C \rightarrow \mathbb{R}$ be a continuously differentiable function. Then f is convex on C if and only if its gradient ∇f is monotone on C , i.e.,

$$\nabla f(x) \cdot (y - x) \leq 0, \quad \forall x, y \in C. \quad (1.6)$$

Proof First we assume that f is a continuously differentiable convex function on C . Let x and $y \in C$, and consider f restricted to the line passing through them, i.e., the function defined by

$$g(t) \triangleq f(x + t(y - x)), \quad (1.7)$$

which, since C is an open convex set and $x, y \in C$, is defined on an open interval I containing $[0, 1]$. Then, by the one-variable characterization Theorem 1.1.16, g is convex on I . Moreover, since g is a continuous differentiable then by Theorem 1.1.1, g' is increasing. Thus we deduce

$$g'(1) \geq g'(0). \quad (1.8)$$

But since

$$g'(t) \triangleq \nabla f(x + t(y - x)) \cdot (y - x), \quad x, y \in C, \quad (1.9)$$

the desired result (1.6) now follows from (1.8).

Conversely, assume that the gradient ∇f is monotone on C and let g be the function defined as in (1.7). Then, for any $t, t_0 \in I$, $0 \leq t - t_0 \leq 1$, we get

$$g(t_0) - g(t) \triangleq \nabla f(x + t_0(y - x)) \cdot (x + t(y - x) - x - t_0(y - x))$$

Let $u \triangleq x + t_0(y - x)$ and $v \triangleq x + t(y - x)$, since u and v are combinations of points in the convex set C then $u, v \in C$. We have $u - v \triangleq (t_0 - t)(y - x)$, then from (1.9) it follows that

$$g(t_0) - g(t) \triangleq (t - t_0) \nabla f(v) \cdot (u - v). \quad (1.10)$$

In view of the monotonicity property (1.6), it follows from (1.10) that g' is non-decreasing. Thus, by Theorem 1.1.1, we deduce that the function g is convex on $[0, 1]$, so from Corollary 1.1.17 the convexity of g on $[0, 1]$ implies the convexity of f on C . ■

Now, we consider the second order characteristic of a twice continuously differentiable convex function. Recall that the second derivative of a real-valued function $f: D \subseteq \mathbb{R}^d \rightarrow \mathbb{R}$ is called a

Hessian matrix, denoted $r^2 f(\mathbf{x})$, with the matrix elements given by:

$$r^2 f(\mathbf{x})_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{x}), i \in 1, \dots, d, j \in 1, \dots, d,$$

provided that f is twice differentiable at $\mathbf{x}$ and the partial derivatives are evaluated at $\mathbf{x}$.

We will now characterize convex functions in terms of their Hessian matrices.

Theorem 1.1.21 (The second-order condition for convexity) *Let $C \subseteq \mathbf{R}^d$ be a nonempty open convex set, and let $f: C \rightarrow \mathbf{R}$ be twice continuously differentiable in C . Then, f is convex on C if and only if $r^2 f(\mathbf{x})$ is positive semi-definite for all $\mathbf{x} \in C$.*

Proof Assume that f is a twice continuously differentiable convex function and let $\mathbf{x} \in C, \mathbf{z} \in \mathbf{R}^d$. Consider again the function of one variable

$$g(t) \in f(\mathbf{x} + t\mathbf{z}), t \in I, \quad (1.11)$$

where $I \in \{t \in \mathbf{R} : \mathbf{x} + t\mathbf{z} \in C\}$. Then as f is a twice differentiable convex function on C , then so is g on I , and, using the fact that

$$g^{(0)}(0) \in \mathbf{z}^T r^2 f(\mathbf{x}) \mathbf{z},$$

which is nonnegative by Theorem 1.1.1, we get that the Hessian of f is positive semi-definite at each $\mathbf{x} \in C$.

For the converse, assume that the Hessian of f is positive semi-definite at each $\mathbf{x} \in C$. Again, using the one-variable characterization of convexity, see Theorem 1.1.16, we need to show convexity of the functions g defined by (1.11). Note that, for all $t \in I$, we have

$$g^{(0)}(t) \in \mathbf{z}^T r^2 f(\mathbf{x} + t\mathbf{z}) \mathbf{z},$$

then the positive semi-definiteness of $r^2 f(\mathbf{x} + t\mathbf{z})$ yields

$$g^{(0)}(t) \geq 0, t \in I.$$

Hence Theorem 1.1.1 confirms that f is a convex function. ■

1.2 Strong convexity and its characterizations

Till now, we have ignored a very important problem: How large is the error between f and its (linear) Taylor approximation. We have seen that the usual convexity implies that the first-order Taylor approximation of f at $\mathbf{x}$, is an under-estimation for the value of f at every other point $\mathbf{y}$. Unfortunately, in general, it is still difficult to get better bounds if we have no

Convex Functions and their Generalizations

additional conditions on f . The first strongest condition that we can impose on f is to belong to the class of strongly convex functions. In particular, it turns out that in this setting, we will obtain much better lower and upper bounds in such an approximation than that from usual convexity, see Corollary 1.2.11 below. Strongly convex functions are defined as follows.

Definition 1.2.1 (Strongly convex function) Let $C \subseteq \mathbb{R}^d$ be a nonempty convex set. A function $f : C \rightarrow \mathbb{R}$ is γ -strongly convex with convexity parameter $\gamma \geq 0$ if, for all $\mathbf{x}, \mathbf{y} \in C$ and all $t \in [0, 1]$ the following holds

$$f(t\mathbf{x} + (1-t)\mathbf{y}) \leq tf(\mathbf{x}) + (1-t)f(\mathbf{y}) - \frac{\gamma}{2}t(1-t)\|\mathbf{x} - \mathbf{y}\|^2.$$

This is a generalization of the concept of (ordinary) convex function. Indeed, if we take $\gamma = 0$, we recover the definition of usual convexity.

Here we state a result concerning the Euclidean norm, which will often be used later.

Lemma 1.2.2 Let $\mathbf{u}, \mathbf{v}$ be in $\mathbb{R}^d$ and $t \in [0, 1]$. Then the following identity holds:

$$\|t\mathbf{u} + (1-t)\mathbf{v}\|^2 \leq t\|\mathbf{u}\|^2 + (1-t)\|\mathbf{v}\|^2 - t(1-t)\|\mathbf{u} - \mathbf{v}\|^2. \quad (1.12)$$

Proof Simple expansions give

$$\begin{aligned} \|t\mathbf{u} + (1-t)\mathbf{v}\|^2 &\leq t^2\|\mathbf{u}\|^2 + 2t(1-t)\langle \mathbf{u}, \mathbf{v} \rangle + (1-t)^2\|\mathbf{v}\|^2 \\ &\leq t(1-t)\|\mathbf{u}\|^2 + 2t(1-t)\langle \mathbf{u}, \mathbf{v} \rangle + (1-t)\|\mathbf{v}\|^2. \end{aligned}$$

The required equality now follows by adding the above two identities and simplifying the resulting expression. ■

The following functions are some important examples of strongly convex functions:

Remark 1.2.3

1. For all $\gamma \geq 0$, $f(\mathbf{x}) = \frac{\gamma}{2}\|\mathbf{x}\|^2$ is a γ -strongly convex function. This is an immediate consequence of Lemma 1.2.2.
2. If each $f_i, i \in 1, 2, \dots, p$ is strongly convex on C , then $\max_{1 \leq i \leq p} f_i$ is also strongly convex on C .
3. Addition of a convex function to a strongly convex function gives a strongly convex function with the same modulus of strong convexity. Therefore, adding a convex function to $\frac{\gamma}{2}\|\mathbf{x}\|^2$ does not affect γ -strong convexity.

Given $\gamma \in \mathbb{R}$ and a nonempty convex set $C \subseteq \mathbb{R}^d$, by $S^\gamma(C)$ we denote the set of all strongly convex functions with convexity parameter γ . As a complement result for Remark 1.2.3, the following result shows that the set $S^\gamma(C)$ is closed under convex combinations.

Proposition 1.2.4 Given a finite family $f_i : i \in 1, \dots, N$ of functions from $S^\gamma(C)$, and given weights $\{w_i\}_{i=1}^N \in [0, 1]$ satisfying $\sum_{i=1}^N w_i = 1$. Then,

$$\sum_{i=1}^N w_i f_i \in S^\gamma(C).$$

Proof Since all $f_i, i \in 1, \dots, N$ are γ -strongly convex, then it holds for any $x, y \in C$, and $t \in [0, 1]$,

$$f_i(t x + (1-t)y) \leq t f_i(x) + (1-t) f_i(y) - \frac{\gamma}{2} t(1-t) \|x - y\|^2.$$

Hence, multiplying both sides of the above inequality by w_i and summing over i yields the required result. ■

1.2.1 Characterizations in terms of usual convexity

The next question is how to characterize the strongly convexity in terms of usual convexity. This question has a remarkably nice answer, there is a very simple and elegant relationship between the two forms of convexity. This important property will be frequently used in the sequel. Indeed, we have the following characterization.

Theorem 1.2.5 Let $C \subseteq \mathbb{R}^d$ be nonempty convex set. A function $f : C \rightarrow \mathbb{R}$ is γ -strongly convex if and only if the function $g \in f + \frac{\gamma}{2} \|\cdot\|^2$ is convex.

Proof Assume that f is strongly convex with convexity parameter γ . Then, by Lemma 1.2.2, we get

$$\begin{aligned} g(t x + (1-t)y) &\leq f(t x + (1-t)y) + \frac{\gamma}{2} \|t x + (1-t)y\|^2 \\ &\leq t f(x) + (1-t) f(y) + \frac{\gamma}{2} t(1-t) \|x - y\|^2 + \frac{\gamma}{2} \|t x + (1-t)y\|^2 \\ &\leq t f(x) + (1-t) f(y) + \frac{\gamma}{2} t \|x\|^2 + \frac{\gamma}{2} (1-t) \|y\|^2 \\ &\leq t g(x) + (1-t) g(y), \end{aligned}$$

which shows that g is convex.

In order to prove the reverse implication, assume that g is convex, then again by Lemma 1.2.2,

we get

$$\begin{aligned} f(t\mathbf{x} + (1-t)\mathbf{y}) &\leq g(t\mathbf{x} + (1-t)\mathbf{y}) + \frac{1}{2} \|t\mathbf{x} - (1-t)\mathbf{y}\|^2 \\ &= tg(\mathbf{x}) + (1-t)g(\mathbf{y}) + \frac{1}{2} t\|\mathbf{x}\|^2 + \frac{1}{2} (1-t)\|\mathbf{y}\|^2 - t(1-t)\|\mathbf{x} - \mathbf{y}\|^2 \\ &= t\left(g(\mathbf{x}) + \frac{1}{2}\|\mathbf{x}\|^2\right) + (1-t)\left(g(\mathbf{y}) + \frac{1}{2}\|\mathbf{y}\|^2\right) - \frac{1}{2}t(1-t)\|\mathbf{x} - \mathbf{y}\|^2 \\ &= tf(\mathbf{x}) + (1-t)f(\mathbf{y}) - \frac{1}{2}t(1-t)\|\mathbf{x} - \mathbf{y}\|^2, \end{aligned}$$

which shows that f is strongly convex with convexity parameter $\frac{1}{2}$. ■

With this result in mind, Proposition 1.2.4 should now be apparent. Also, from the above characterization, we can now state the following observation.

Remark 1.2.6 *It is clear from the definitions that strong convexity implies usual convexity, but the converse is not true in general. For example, the function f defined by*

$$f(x) \triangleq x^4, \quad 1 \leq x \leq 1,$$

is convex but is not strongly convex. To show this, assume, to the contrary, that f is strongly convex on $I \triangleq [1, 1]$. Then, by Theorem 1.2.5, there exists a convex function g and a scalar $\epsilon > 0$ such that for any $x \in I$, function f can be expressed as

$$f(x) \triangleq g(x) + \frac{\epsilon}{2} x^2.$$

But then, at $x = 0$, we must clearly have

$$0 \leq f''(0) \leq g''(0) + \epsilon,$$

and therefore $g''(0) \leq -\epsilon < 0$. This is a contradiction since we know that by the classical second-order characterization of convexity, see Theorem 1.1.21, $g''(0) \geq 0$. Hence, f is not strongly convex on I . In fact, a similar argument may be used to show that for any $p \in \mathbb{Z}$ the function $f_p(x) \triangleq x^p$ is convex but not strongly convex on I .

1.2.2 Uniqueness of minimum for strongly convex functions

The following theorem illustrates why strongly convex functions are of fundamental importance in optimization. It shows that strong convexity is sufficient to guarantee the uniqueness of minimizers. The concepts of the strongly convex functions have played very important role in the development of convex programming, see [6]. Relaxation of ordinary convexity by imposing a restricted strong convexity condition is also commonly used in economic models, see, e. g., [11].

Theorem 1.2.7 (Uniqueness of Global minimum) Let $f: C \rightarrow \mathbb{R}$ be a strongly convex function defined on a convex set $C \subseteq \mathbb{R}^d$. Then f attains its minimum, at most, one point.

Proof Assume to the contrary that the set of minimal points M is not empty and contains two distinct points $\mathbf{x}$ and $\mathbf{y}$. Then, for any $0 \leq \lambda \leq 1$, since M is convex, we have $(1-\lambda)\mathbf{x} + \lambda\mathbf{y} \in M$. But f is strongly convex, hence

$$\begin{aligned} f((1-\lambda)\mathbf{x} + \lambda\mathbf{y}) &\leq f((1-\lambda)\mathbf{x} + \lambda\mathbf{y}) \leq (1-\lambda)f(\mathbf{x}) + \lambda f(\mathbf{y}) - \frac{\lambda(1-\lambda)}{2} \|\mathbf{x} - \mathbf{y}\|^2 \\ &\leq f(\mathbf{x}) - \frac{\lambda(1-\lambda)}{2} \|\mathbf{x} - \mathbf{y}\|^2 < f(\mathbf{x}), \end{aligned}$$

which is a contradiction. ■

1.2.3 The first-order condition for strongly convex functions

When the function is differentiable, an alternative characterization of strong convexity is in terms of the gradient inequality. Geometrically, the following theorem means that at any $\mathbf{x} \in C$, there exists a convex quadratic function

$$f_{\text{low}}(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) - \frac{\lambda}{2} \|\mathbf{x} - \mathbf{y}\|^2,$$

that bounds from below the graph of f , that is such that

$$f(\mathbf{y}) \geq f_{\text{low}}(\mathbf{y}),$$

holds for all $\mathbf{y} \in C$. It is obviously seen that this lower bound is better than its first order (linear) approximation, which is implied by usual convexity. Indeed, we always have the following inequalities

$$f(\mathbf{y}) \geq f_{\text{low}}(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}).$$

Theorem 1.2.8 Let f be a continuously differentiable function defined on an open convex set $C \subseteq \mathbb{R}^d$. Then f is strongly convex with parameter $\lambda \geq 0$ if and only if for any $\mathbf{x}, \mathbf{y} \in C$ we have

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) - \frac{\lambda}{2} \|\mathbf{x} - \mathbf{y}\|^2. \quad (1.13)$$

Proof Let f be strongly convex on C with parameter λ , then for any $\mathbf{x}, \mathbf{y} \in C$

$$f(t\mathbf{y} + (1-t)\mathbf{x}) \leq tf(\mathbf{y}) + (1-t)f(\mathbf{x}) - \frac{\lambda}{2} t(1-t) \|\mathbf{x} - \mathbf{y}\|^2.$$

Hence

$$tf(\mathbf{y}) + (1-t)f(\mathbf{x}) \geq f(t\mathbf{y} + (1-t)\mathbf{x}) + \frac{\lambda}{2} t(1-t) \|\mathbf{x} - \mathbf{y}\|^2,$$

but then

$$tf(y) - f(x) - t(f(x) - f(y)) \leq t(1-t) \|x - y\|^2.$$

$$t(f(y) - f(x)) \leq t(1-t) \|x - y\|^2.$$

Dividing the above inequality by t gives

$$f(y) - f(x) \leq (1-t) \|x - y\|^2.$$

Therefore, letting $t \neq 0$ yields the desired result (1.13). To prove the converse implication, let us assume that (1.13) holds. Let us fix $x, y \in C$, $t \in [0, 1]$, and write $z = tx + (1-t)y$. Then

$$f(z) \leq f(x) + t(f(y) - f(x)),$$

it can be expressed as

$$f(z) \leq f(x) + t(f(y) - f(x)),$$

or equivalently as

$$f(z) \leq t f(x) + (1-t) f(y),$$

hence identity (1.13) implies

$$f(z) - t f(x) - (1-t) f(y) \leq 0. \quad (1.14)$$

This can be rewritten as

$$f(z) - t f(x) - (1-t) f(y) \leq 0. \quad (1.15)$$

On the other hand, by Lemma 1.2.2 and making the substitutions

$$u = x - z$$

$$v = y - z$$

$$u + v = x - y$$

$$tu + (1-t)v = 0,$$

we get

$$0 \leq t \|x - z\|^2 + (1-t) \|y - z\|^2 - t(1-t) \|x - y\|^2.$$

This identity, combined with (1.15), implies that f is t -strongly convex as required.

Another and direct proof consists of observing that by Theorem 1.2.5 the function $g \in f + \frac{1}{2}k^2$ is still convex, and thus to obtain (1.13), it is enough to apply the first-order condition for convexity to the function g , see Theorem 1.1.18. ■

1.2.4 Characterization via the strong monotonicity of the gradient

Theorem 1.2.9 *Let f be a continuously differentiable function defined on an open convex set $C \subset \mathbb{R}^d$. Then f is strongly convex with parameter $\gamma \geq 0$ if and only if its gradient ∇f is uniformly monotone i.e.,*

$$\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq \gamma \|x - y\|^2, \quad x, y \in C. \quad (1.16)$$

Proof Let f be γ -strongly convex on C , and let $x, y \in C$. Define $g \in f + \frac{1}{2}\gamma\|x - y\|^2$, and note that $\nabla g(x) = \nabla f(x) + \gamma(x - y)$ hence

$$\langle \nabla f(x) - \nabla f(y), x - y \rangle \leq \langle \nabla g(x) - \nabla g(y), x - y \rangle.$$

Thus, since f is γ -strongly convex, then by Theorem 1.2.5 g is a convex function, and so it follows

$$\begin{aligned} \langle \nabla f(x) - \nabla f(y), x - y \rangle &\leq \langle \nabla g(x) - \nabla g(y), x - y \rangle \\ &\leq \frac{1}{2} \gamma \|x - y\|^2. \end{aligned} \quad (1.17)$$

This shows that the desired inequality (1.16) is satisfied.

Conversely, assume that (1.16) holds. Then, from identity (1.17) we deduce, for all $x \in C$,

$$\langle \nabla g(x) - \nabla g(y), x - y \rangle \geq 0, \quad (1.19)$$

which shows that ∇g is monotone on C . Therefore by Theorem 1.1.20 it follows that g is convex. Now Theorem 1.2.5 implies that f is strongly convex. ■

Let C be a non-empty convex open subset of $\mathbb{R}^d$. By $S^1_\gamma(C)$, we denote the set of all continuously differentiable strongly convex functions with convexity parameter $\gamma \geq 0$.

The following theorem complements the results of Theorems 1.2.8 and 1.2.9, providing, in particular, a way to find an upper bound on the error in the (linear) Taylor approximation of a strongly convex function.

Theorem 1.2.10 *If $f \in S^1_\gamma(C)$, then for any x and y from C we have*

$$f(y) - f(x) - \langle \nabla f(x), y - x \rangle \leq \frac{1}{2} \gamma \|y - x\|^2, \quad (1.20)$$

$$h(x) = f(y) + \frac{1}{2} \|x - y\|^2. \quad (1.21)$$

Proof Let us fix some point $x \in C$ and consider the function g defined for all $y \in C$ by

$$g(y) = f(y) + h(x).$$

Since $h(x, \cdot)$ is an affine function and is therefore convex, then by Remark 1.2.3 $g \in S^1(C)$. Thus Theorem 1.2.8 guarantees that for any $y, v \in C$ we have

$$g(v) \geq g(y) + \langle \nabla g(y), v - y \rangle + \frac{1}{2} \|v - y\|^2. \quad (1.22)$$

We observe that for any $y \in C$

$$\begin{aligned} \nabla g(y) &= \nabla f(y) + \nabla h(x), \\ \nabla g(x) &= 0. \end{aligned}$$

Since g is also convex on C , it attains its global minimum at the critical point x , see Theorem 1.1.13. In light of inequality (1.22) for any $y \in C$, there holds

$$g(x) \leq \min_{v \in C} g(v) \leq \min_{v \in C} h(v),$$

where h is the function defined on C by

$$h(v) = g(y) + \langle \nabla g(y), v - y \rangle + \frac{1}{2} \|v - y\|^2.$$

Since h is convex, then it attains its global minimum over C at its critical point $v \in C$ such that $\nabla h(v) = 0$. Then we conclude that

$$\begin{aligned} g(x) &\leq g(y) + \langle \nabla g(y), x - y \rangle + \frac{1}{2} \|x - y\|^2 \\ &= g(y) + \frac{1}{2} \langle \nabla g(y), x - y \rangle + \frac{1}{2} \|x - y\|^2 \\ &= g(y) + \frac{1}{2} \langle \nabla g(y), x - y \rangle + \frac{1}{2} \|x - y\|^2 \\ &= g(y) + \frac{1}{2} \langle \nabla g(y), x - y \rangle + \frac{1}{2} \|x - y\|^2 \\ &= g(y) + \frac{1}{2} \langle \nabla g(y), x - y \rangle + \frac{1}{2} \|x - y\|^2 \\ &= g(y) + \frac{1}{2} \langle \nabla g(y), x - y \rangle + \frac{1}{2} \|x - y\|^2. \end{aligned}$$

Thus we have shown that

$$g(x) \leq g(y) + \frac{1}{2} \|\nabla g(y)\|^2,$$

which is exactly the desired inequality (1.20).

By switching the role of x and y in (1.20), we finally get, by adding and rearranging, the required inequality 1.21. ■

1.2. Strong convexity and its characterizations

To understand the usefulness of strong convexity, note that by Theorems 1.2.8 and 1.2.10 it provides better error estimates in the linear approximation

$$R[f](\mathbf{x}, \mathbf{y}) \leq f(\mathbf{y}) - f(\mathbf{x}) - \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}).$$

Indeed, these theorems allow us to control the error $R[f]$ as follows.

Corollary 1.2.11 *Let f be a continuously differentiable function defined on an open convex set $C \subset \mathbb{R}^d$. Then the following assertions hold true:*

1. *f is convex on C then for all $\mathbf{x}, \mathbf{y} \in C$ there holds $R[f](\mathbf{x}, \mathbf{y}) \geq 0$.*
2. *f is μ -strongly convex on C then for all $\mathbf{x}, \mathbf{y} \in C$ there holds*

$$-\frac{\mu}{2} \|\mathbf{x} - \mathbf{y}\|^2 \leq R[f](\mathbf{x}, \mathbf{y}) \leq \frac{\mu}{2} \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|^2.$$

1.2.5 The second-order condition for strongly convex functions

Strong convexity can also be characterized by a second-order condition.

Theorem 1.2.12 *Let $C \subset \mathbb{R}^d$ be a nonempty open convex set, and let $f: C \rightarrow \mathbb{R}$ be twice continuously differentiable in C . Then f is strongly convex with parameter $\mu \geq 0$ if and only if for all $\mathbf{x} \in C, \mathbf{y} \in \mathbb{R}^d$*

$$-\mu \|\mathbf{y}\|^2 \leq \nabla^2 f(\mathbf{x})[\mathbf{y}, \mathbf{y}], \quad \mathbf{x} \in C, \mathbf{y} \in \mathbb{R}^d. \quad (1.23)$$

◦ ◦

Proof Let f be strongly convex on C with parameter μ , then again, Theorem 1.2.5 says that the function $g \in f - \frac{\mu}{2} \|\cdot\|^2$ is convex, and thus its Hessian matrix is positive semi-definite

$$-\mu \|\mathbf{y}\|^2 \leq \nabla^2 g(\mathbf{x})[\mathbf{y}, \mathbf{y}], \quad \mathbf{x} \in C, \mathbf{y} \in \mathbb{R}^d. \quad (1.24)$$

But we have

$$\nabla^2 g(\mathbf{x})[\mathbf{y}, \mathbf{y}] = \nabla^2 f(\mathbf{x})[\mathbf{y}, \mathbf{y}] - \mu \|\mathbf{y}\|^2,$$

◦ ◦

and finally positive definiteness of $\nabla^2 g$ yields the desired inequality (1.23).

To prove the converse, let us fix $\mathbf{x} \in C, \mathbf{y} \in C$. By Taylor's Theorem we have

$$f(\mathbf{y}) - f(\mathbf{x}) = \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) + \frac{1}{2} \nabla^2 f(\xi) (\mathbf{y} - \mathbf{x})^T (\mathbf{y} - \mathbf{x})$$

for some $\xi \in [0, 1]$. Clearly, if the Hessian satisfies (1.23), then we obtain the first-order condition for strong convexity of f . Thus, Theorem 1.2.8 implies that f is strongly convex on C . ■

1.3 Convex functions with Lipschitz continuous gradients

In order to obtain better bounds for the linear approximation, instead of strong convexity, now consider the case when the gradient is Lipschitz continuous. In this setting, we will also get better bounds, see Theorem 1.3.4 below.

1.3.1 Lipschitz-continuous gradient

Definition 1.3.1 (L -Lipschitz-continuous gradient) Let D be an open subset of $\mathbf{R}^d$. A differentiable function $f: D \rightarrow \mathbf{R}$ has a Lipschitz-continuous gradient with constant $L \geq 0$ if and only if

$$\| \nabla f(\mathbf{x}) - \nabla f(\mathbf{y}) \| \leq L \|\mathbf{x} - \mathbf{y}\|, \quad \forall \mathbf{x}, \mathbf{y} \in D. \quad (1.25)$$

If the gradient of f is Lipschitz-continuous, we can obtain quadratic upper and lower bounds on the function. This result, known as “the descent lemma,” is fundamental in convergence proofs of gradient-based methods.

Theorem 1.3.2 (quadratic upper and lower bounds) Let f be a differentiable function defined on an open set $C \subset \mathbf{R}^d$. Assume that ∇f is Lipschitz-continuous with constant L , then $\forall \mathbf{x}, \mathbf{y} \in C$

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) + \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|^2$$

Proof By the fundamental theorem for line integrals,

$$f(\mathbf{y}) - f(\mathbf{x}) = \int_0^1 \nabla f(\mathbf{x} + t(\mathbf{y} - \mathbf{x}))^T (\mathbf{y} - \mathbf{x}) dt.$$

Therefore

$$f(\mathbf{y}) - f(\mathbf{x}) - \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) = \int_0^1 (\nabla f(\mathbf{x} + t(\mathbf{y} - \mathbf{x})) - \nabla f(\mathbf{x}))^T (\mathbf{y} - \mathbf{x}) dt.$$

Then it holds that

$$\begin{aligned}
 |f(\mathbf{y}) - f(\mathbf{x}) - \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle| &= \left| \int_0^1 \langle \nabla f(\mathbf{x} + t(\mathbf{y} - \mathbf{x})) - \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle dt \right| \\
 &\leq \|\mathbf{y} - \mathbf{x}\| \int_0^1 \|\nabla f(\mathbf{x} + t(\mathbf{y} - \mathbf{x})) - \nabla f(\mathbf{x})\| dt \\
 &\leq \|\mathbf{y} - \mathbf{x}\| \int_0^1 L \|\mathbf{y} - \mathbf{x}\| dt \\
 &= \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|^2.
 \end{aligned}$$

■

Note that the proof of the theorem actually shows both upper and lower bounds on the function.

Theorem 1.3.3 (Characterization of quadratic upper bound) Let f be a differentiable function defined on an open convex set $C \subseteq \mathbb{R}^d$. Assume that ∇f is Lipschitz-continuous with constant L , then the following properties hold and follow from each other.

- (1) The function $g(\mathbf{x}) = \frac{L}{2} \|\mathbf{x}\|^2 + f(\mathbf{x})$ is convex on C .
- (2) The function f satisfies the upper bound property:

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|^2, \quad (\mathbf{x}, \mathbf{y} \in C). \quad (1.26)$$

Proof Cauchy-Schwarz inequality and Lipschitz continuity of ∇f imply

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y}\| \leq L \|\mathbf{y} - \mathbf{x}\|^2, \quad (1.27)$$

and since $f(\mathbf{x}) = \frac{L}{2} \|\mathbf{x}\|^2 + g(\mathbf{x})$, we deduce that

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y}\| \leq L \|\mathbf{y} - \mathbf{x}\|^2 + \langle \nabla g(\mathbf{x}) - \nabla g(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle. \quad (1.28)$$

Inserting this into (1.27) yields

$$\langle \nabla g(\mathbf{x}) - \nabla g(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \geq 0. \quad (1.29)$$

Hence, by Theorem 1.1.20, we can conclude that g is indeed convex.

Furthermore, by Theorem 1.3.2, it follows that f satisfies the upper bound property (1.26).

Next we show that (1) and (2) are equivalent. Since $\nabla f(\mathbf{x}) = L\mathbf{x} + \nabla g(\mathbf{x})$ and consequently

$$\langle \nabla f(\mathbf{x}), \mathbf{x} - \mathbf{y} \rangle = L \|\mathbf{x} - \mathbf{y}\|^2 + \langle \nabla g(\mathbf{x}), \mathbf{x} - \mathbf{y} \rangle, \quad \text{⑧}$$

note also that the following holds true:

$$\frac{1}{2} \|y\|^2 \leq \frac{1}{2} \|x\|^2 + \langle x, y \rangle + \frac{1}{2} \|x - y\|^2,$$

then substituting in (1.26), and then rearranging we obtain that the upper bound property is equivalent to the first order condition for convexity of g ,

$$g(x) \leq h g(x), y \mid x \cdot g(y), (x, y \in C).$$

Hence, the two properties are equivalent. ■

1.3.2 Sandwiching smooth convex functions

In the case of convex function, we can use the first-order property to lower bound f

$$f(x) \geq h f(x), y \mid x \cdot f(y).$$

Moreover, if f has L -Lipschitz continuous gradient, then we can use the upper bound property, to upper bound f

$$f(y) \leq f(x) + h f(x), y \mid x \leq \frac{L}{2} \|y - x\|^2. \quad (1.30)$$

Hence, combining convexity and using L -Lipschitz continuity of the gradient, we get the following error estimates for the linear approximation

$$0 \leq f(y) - f(x) - h f(x), y \mid x \leq \frac{L}{2} \|y - x\|^2. \quad (1.31)$$

The following result gives a better lower bound of f than in (1.31) using the quantity $\|h f(x) - r f(y)\|$. It also provides error estimates in the linear approximation for convex, differentiable functions with Lipschitz continuous gradients.

Theorem 1.3.4 (Co-coercivity of gradient) Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be a differentiable convex with L -Lipschitz continuous gradient ($L \geq 0$), then for all $x, y \in \mathbb{R}^d$

$$\frac{1}{2L} \|h f(x) - r f(y)\|^2 \leq f(y) - f(x) - h f(x), y \mid x \leq \frac{L}{2} \|y - x\|^2. \quad (1.32)$$

Proof By Theorem 1.3.2, it remains to prove the left inequality. Let $x, y, z \in \mathbb{R}^d$. Let us approximate $f(z)$ from below by $f(y)$ and from above by $f(x)$, respectively. Using (1.31), then it holds that

$$f(z) - f(x) - h f(x), z \mid x \geq 0, \quad (1.33)$$

$$f(z) - f(y) - h f(y), z \mid y \leq \frac{L}{2} \|z - y\|^2. \quad (1.34)$$

Multiplying inequality (1.33) by α and adding it to the inequality (1.34), we get

$$f(\mathbf{x}) - f(\mathbf{y}) \leq \alpha \langle \mathbf{g}(\mathbf{x}), \mathbf{z} - \mathbf{x} \rangle + \alpha \langle \mathbf{g}(\mathbf{y}), \mathbf{z} - \mathbf{y} \rangle + \frac{L}{2} \|\mathbf{z} - \mathbf{y}\|^2.$$

The above inequality can also be written as

$$\langle \mathbf{g}(\mathbf{x}), \mathbf{z} - \mathbf{y} \rangle + \langle \mathbf{g}(\mathbf{y}), \mathbf{z} - \mathbf{y} \rangle \leq \frac{L}{2} \|\mathbf{z} - \mathbf{y}\|^2 + f(\mathbf{y}) - f(\mathbf{x}) + \langle \mathbf{g}(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle.$$

Let us take $\mathbf{z} = \mathbf{y} + \alpha(\mathbf{g}(\mathbf{x}) - \mathbf{g}(\mathbf{y}))$ for any $\alpha \in \mathbb{R}$, then it follows from the above inequality

$$\mu_\alpha \leq \frac{\alpha^2 L}{2} \|\mathbf{g}(\mathbf{x}) - \mathbf{g}(\mathbf{y})\|^2 + f(\mathbf{y}) - f(\mathbf{x}) + \langle \mathbf{g}(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle, \quad (\forall \alpha \in \mathbb{R}).$$

Now, the desired result follows since the lower bound is a concave quadratic function in α , then its maximum value is attained at stationary point $\alpha = 1/L$. ■

1.3.3 Error estimates for linear approximation

Combining Theorem 1.3.4 with Corollary 1.2.11, the following result tells us that if a function has both strong convexity and Lipschitz assumption of its gradient, the linear approximation may be bounded both from below and above by quadratic functions.

Theorem 1.3.5 Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be a differentiable μ -strongly convex function with L -Lipschitz continuous gradient ($L \geq 0$), then for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$

$$\frac{1}{2L} \|\mathbf{g}(\mathbf{x}) - \mathbf{g}(\mathbf{y})\|^2 + f(\mathbf{y}) - f(\mathbf{x}) + \langle \mathbf{g}(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \leq \frac{1}{2\mu} \|\mathbf{g}(\mathbf{x}) - \mathbf{g}(\mathbf{y})\|^2 \quad (1.35)$$

$$\frac{1}{2L} \|\mathbf{g}(\mathbf{x}) - \mathbf{g}(\mathbf{y})\|^2 + f(\mathbf{y}) - f(\mathbf{x}) + \langle \mathbf{g}(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \leq \frac{L}{2} \|\mathbf{x} - \mathbf{y}\|^2. \quad (1.36)$$

1.3.4 Characterization of Lipschitz continuity of the gradient

We need a property of the gradient called *co-coercivity*.

Definition 1.3.6 (Co-coercive mapping) A mapping $F : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is co-coercive with parameter c if for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$,

$$\langle F(\mathbf{x}) - F(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \geq c \|\mathbf{x} - \mathbf{y}\|^2. \quad (1.37)$$

The next result offers simple ways to characterize differentiable functions with Lipschitz continuous gradients.

Theorem 1.3.7 Let f be a differentiable convex function defined on $\mathbb{R}^d$. Then the following properties are equivalent.

(1) rf is Lipschitz-continuous with constant L .

(2) The function f satisfies for all $\mathbf{x}, \mathbf{y} \in \mathbf{R}^d$

$$f(\mathbf{x}) - \langle \mathbf{r}f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \leq f(\mathbf{y}) \leq f(\mathbf{x}) + \langle \mathbf{r}f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|^2. \quad (1.38)$$

(3) The function f satisfies for all $\mathbf{x}, \mathbf{y} \in \mathbf{R}^d$

$$\frac{1}{2L} \|\mathbf{r}f(\mathbf{x}) - \mathbf{r}f(\mathbf{y})\|^2 \leq f(\mathbf{x}) - \langle \mathbf{r}f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \leq f(\mathbf{y}). \quad (1.39)$$

(4) rf is co-coercive mapping with constant $\frac{1}{L}$. That is

$$\langle \mathbf{r}f(\mathbf{x}) - \mathbf{r}f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \geq \frac{1}{L} \|\mathbf{r}f(\mathbf{x}) - \mathbf{r}f(\mathbf{y})\|^2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbf{R}^d. \quad (1.40)$$

Proof By Theorems 1.3.2 and 1.3.4, it remains to show that

$$(3) \Rightarrow (4), \text{ and } (4) \Rightarrow (1).$$

Assume that (3) holds, then for all $\mathbf{x}, \mathbf{y} \in \mathbf{R}^d$, we have

$$\frac{1}{2L} \|\mathbf{r}f(\mathbf{x}) - \mathbf{r}f(\mathbf{y})\|^2 \leq f(\mathbf{y}) - f(\mathbf{x}) \leq \langle \mathbf{r}f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle. \quad (1.41)$$

Similarly, but with the roles of $\mathbf{x}$ and $\mathbf{y}$ interchanged, we have

$$\frac{1}{2L} \|\mathbf{r}f(\mathbf{x}) - \mathbf{r}f(\mathbf{y})\|^2 \leq f(\mathbf{x}) - f(\mathbf{y}) \leq \langle \mathbf{r}f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle. \quad (1.42)$$

Then, by adding inequalities (1.41) and (1.42), the co-coercivity of rf with constant $1/L$ follows.

Finally, assume that rf is co-coercive with constant $1/L$. Then the Cauchy-Schwarz inequality, applied to the left-hand side of (1.40), implies that rf is Lipschitz continuous with Lipschitz constant L . ■

1.3.5 Strong convex functions with Lipschitz continuous derivatives

Definition 1.3.8 Let ϵ be a positive number. A differentiable function $f: C \rightarrow \mathbf{R}$ with a convex domain C belongs to the class $S^{\epsilon,L}(C)$ if f is ϵ -strongly convex and the gradient rf is Lipschitz continuous with Lipschitz constant L . The quotient $Q \in \mathbf{R}^+$ is called the condition number of the class $S^{\epsilon,L}(C)$.

1.3. Convex functions with Lipschitz continuous gradients

If we know that f belongs to the class $S_{\mu,L}^1(C)$, then due to Theorem 1.2.9 f satisfies the following two inequalities for all $\mathbf{x}, \mathbf{y} \in C$:

$$f(\mathbf{x}) - f(\mathbf{y}) \leq \langle \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle + \frac{L}{2} \|\mathbf{x} - \mathbf{y}\|^2, \quad (1.43)$$

$$f(\mathbf{x}) - f(\mathbf{y}) \geq \langle \nabla f(\mathbf{x}), \mathbf{x} - \mathbf{y} \rangle - \frac{\mu}{2} \|\mathbf{x} - \mathbf{y}\|^2. \quad (1.44)$$

Using Cauchy-Schwarz inequality on the first term of (1.43), we obtain the inequality $\langle \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \leq \|\nabla f(\mathbf{y})\| \|\mathbf{x} - \mathbf{y}\|$, then according to (1.44) we conclude that $\mu \leq L$ and therefore the condition number $Q = \frac{L}{\mu} \geq 1$. Hence, μ should be less than or equal to L if the function is both μ -strongly convex and its gradient is L -Lipschitz continuous.

1.3.6 Co-coercivity property for strongly convex functions

The next result is a co-coercivity version for strongly convex functions. Its proof is based on Theorem 1.3.7.

Theorem 1.3.9 If $f \in S_{\mu,L}^1(\mathbb{R}^d)$, then

$$\langle \nabla f(\mathbf{x}) - \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \geq \frac{\mu}{L} \|\mathbf{x} - \mathbf{y}\|^2 \geq \frac{1}{L^2} \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|^2 \quad (1.45)$$

for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.

Proof Let $f \in S_{\mu,L}^1(\mathbb{R}^d)$. Define

$$g(\mathbf{x}) \triangleq f(\mathbf{x}) - \frac{\mu}{2} \|\mathbf{x}\|^2, \quad (1.46)$$

then

$$\langle \nabla g(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \leq \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle - \mu \langle \mathbf{x}, \mathbf{y} - \mathbf{x} \rangle.$$

Hence, in view of Theorem 1.3.2 we get

$$\begin{aligned} g(\mathbf{y}) &\leq f(\mathbf{y}) - \frac{\mu}{2} \|\mathbf{y}\|^2 \\ &\leq f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|^2 - \frac{\mu}{2} \|\mathbf{y}\|^2 \\ &\leq g(\mathbf{x}) + \frac{\mu}{2} \|\mathbf{x}\|^2 + \langle \nabla g(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|^2 - \frac{\mu}{2} \|\mathbf{y}\|^2 \\ &\leq g(\mathbf{x}) + \langle \nabla g(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|^2. \end{aligned}$$

On the other hand we have (again from convexity)

$$g(x) \leq hrg(x, y) \leq g(y), \quad (1.47)$$

then we get the following bounds

$$g(x) \leq hrg(x, y) \leq g(y) \leq g(x) \leq hrg(x, y) \leq \frac{L}{L+1} \|y-x\|^{L+1}. \quad (1.48)$$

This shows that g satisfies condition (2) of Theorem 1.3.7 with $L+1$ instead of L . Then, rg is Lipschitz continuous with constant $L+1$. If $L+1 \neq 0$, then it follows from equation (1.48) that

$$g(y) \leq g(x) \leq hrg(x, y) \leq g(y). \quad (1.49)$$

Since x, y are arbitrary in (1.49), then there exists a constant vector $a \in \mathbb{R}^d$ such that for all $y \in \mathbb{R}^d$, $rg(x) \leq a$. This means that g is an affine function:

$$g(y) \leq a, y \leq c,$$

where c is some real constant. Now from (1.46), we deduce that f is a quadratic polynomial of the form

$$f(y) \leq \frac{1}{2} \|y\|^2 \leq a, y \leq c. \quad (1.50)$$

A simple inspection shows that inequality (1.45) holds for all quadratic polynomials of the form (1.50).

We now prove that (1.45) is also valid if $L \neq 1$. Again we can apply Theorem 1.3.7, condition (4), to get that rg is co-coercive with constant $\frac{1}{L+1}$, which means

$$hrg(x) \leq rg(y), x \leq y, \quad \frac{1}{L+1} \|rg(x) - rg(y)\|^2, \quad (1.51)$$

this, by the definition of g , is of course just a reformulation of the required result (this is ensured by the transformation (1.46)). ■

In particular, for $L \neq 0$, we obtain the usual co-coercivity property for convex functions.



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2 Approximations of differentiable convex functions on arbitrary convex polytopes

We begin this chapter with giving two equivalent definitions of a prototype and then state some well-known fundamental theorems and properties of such a geometric object. In Section 2.2, we define the notion of generalized barycentric coordinates with respect to an arbitrary set of points in $\mathbf{R}^d$, or equivalently, with respect to a (convex) polytope. We then show that such coordinates always exist for any finite point set. This existence result is due to Kalman in the sixties [26, Theorem 2]. Section 2.2 also introduces Delaunay triangulation as duals of Voronoi diagrams. It summarizes basic properties of such a widely-used triangulation. Under the convexity assumption, Section 2.3 provides an approximation method, which we call it a barycentric approximation. This class of (linear) operators approximate all convex functions from above. We then give a characterization result for these operators in terms of their error estimates. Such a characterization theorem is due to Guessab in his recent paper [2].

2.1 Convex polytopes

Convex polytopes are fundamental geometric objects. To a large degree or widely the geometry of polytopes is just that of $\mathbf{R}^d$ itself. In the following, we give two different versions of the definition of a polytope. (We speak of *polytopes* without including the word *convex*, we do not consider non-convex polytopes). The two versions are mathematically, but not algorithmically, equivalent. The proof of equivalence between the two concepts is nontrivial, see [12, Lecture 1]. The two concepts have also proved to be fundamental in a new field called “computational convexity”; see [27, 28]

Definition 2.1.1 (polytope) A $\mathbb{R}^d$ polytope is the convex hull of a finite set of points in some $\mathbf{R}^d$. An H polyhedron is an intersection of finitely many closed halfspaces in some $\mathbf{R}^d$. An H polytope is an H polyhedron that is bounded in the sense that it does not contain a ray

$\{x \in \mathbb{R}^d : t \leq y \leq 0\}$ for any $y \in \mathbb{R}^d$.

This definition of 'bounded' has the advantage over others that it does not rely on a metric or scalar product, and that it is obviously invariant under affine change of coordinates. The second concept, an H -polyhedron, denotes an intersection of closed halfspaces: a set $P \subseteq \mathbb{R}^d$ presented in the form

$$P = \{x \in \mathbb{R}^d : Ax \leq z\} \text{ for some } A \in \mathbb{R}^{m \times d}, z \in \mathbb{R}^m.$$

Here " $Ax \leq z$ " is the shorthand for a system of inequalities, namely $a_1 \cdot x \leq z_1, \dots, a_m \cdot x \leq z_m$, where $a_1, \dots, a_m$ are the rows of A , and $z_1, \dots, z_m$ are the components of z .

A compact convex set $K \subseteq \mathbb{R}^d$ is a polytope provided $\text{ext}K$ (the set of all extreme points of K) is a finite set. From the results of [11, section 2.4 and theorem 2.3.4] it follows that polytopes may equivalently be defined as convex hulls of finite sets. For a polytope K , it is customary to call the points of $\text{ext}K$ *vertices*. We denote them by $\text{vert}K$.

The dimension of a polytope is the dimension of its affine hull. A d -polytope is a polytope of dimension d in some $\mathbb{R}^e$ ($e \geq d$).

For examples, zero-dimensional polytopes are points, one-dimensional polytopes are line segments, two-dimensional polytopes are called *polygons*. A polygon with n vertices is called an n -gon. Convexity here requires that the interior angles (at the vertices) are all smaller than π . The following drawing shows a convex 6-gon, or *hexagon*, also, the *tetrahedron* is a familiar geometric object (a 3-dimensional polytope) in $\mathbb{R}^3$. Similarly, its d -dimensional generalization forms the first (and simplest) infinite family of higher-dimensional polytopes we want to consider.

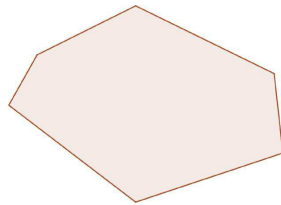
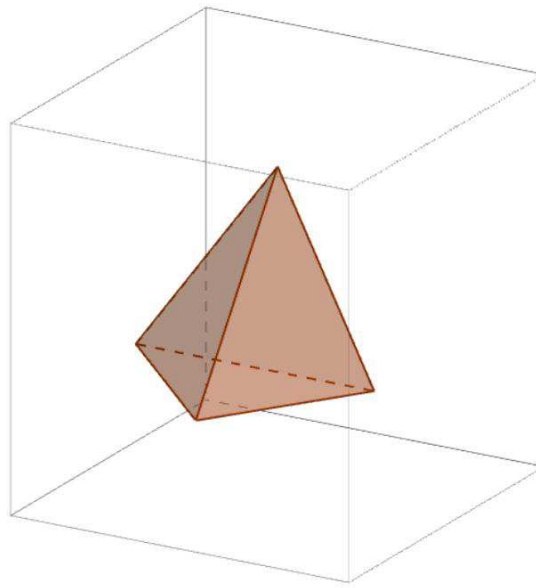


Figure 2.1 – 6-gon or hexagon.

Figure 2.2 – the tetrahedron in $\mathbf{R}^3$.

Our following sketches try to illustrate the two concepts: the left figure shows a pentagon constructed as a $\mathcal{V}_1$ polytope as the convex hull of five points; the right figure shows the same pentagon as an $\mathcal{H}_1$ polytope, constructed by intersecting five lightly shaded halfspaces (bounded by the five fat lines). Usually we assume (without loss of generality) that the polytopes we study are full-dimensional, so that d denotes both the dimension of the polytope we are studying, and the dimension of the ambient space $\mathbf{R}^d$.

Figure 2.3 – Polytope which presented in two ways either as a $\mathcal{V}_1$ polytope or as an $\mathcal{H}_1$ polytope.

2.1.1 Fundamental theorems and properties of polytopes

One of the main tasks for polytope theory is to develop tools to analyze and, if possible, *visualize* the geometry of higher-dimensional polytopes. Now we start with a basic version of the *representation theorem for polytopes*. See [12, Theorem 1.1]

Theorem 2.1.2 (Main theorem for polytopes) *A subset $P \subset \mathbb{R}^d$ is the convex hull of a finite point set (a polytope) if and only if it is a bounded intersection of halfspaces (a polytope)*

$$P \in \text{conv}(V) \text{ for some } V \subset \mathbb{R}^d,$$

if and only if it is a bounded intersection of halfspaces (a polytope)

$$P \in P(A, z) \text{ for some } A \subset \mathbb{R}^d, z \in \mathbb{R}^d.$$

This result contains two implications, which are equally (geometrically clear) and which in a certain sense are equivalent. This theorem is important because it provides two independent characterizations of polytopes that are of different power, depending on the problem we are studying. For example, consider the following four statements.

- Every intersection of a polytope with an affine subspace is a polytope.
- Every intersection of a polytope with a polyhedron is a polytope.
- Every projection of a polytope is a polytope.
- The Minkowski sum of two polytopes is polytope,
where the vector sum (or Minkowski sum) of two sets $P, Q \subset \mathbb{R}^d$ is defined to be

$$P \dot{+} Q := \{x \dot{+} y : x \in P, y \in Q\}.$$

The first two statements are trivial for a polytope presented in the form $P \in P(A, z)$ (where the first is a special case of the second), but both are nontrivial for the convex hull of a finite set of points. Similarly the last two statements are easy to see for the convex hull of a finite point set, but are nontrivial for bounded intersections of halfspaces.

For more details about the proofs of the following theorem and its corollary see [13, Theorem 2.8 and corollary 2.9].

Theorem 2.1.3 *For any compact subset M of $\mathbb{R}^d$, the convex hull $\text{conv}(M)$ is again compact.*

Since any finite set is compact, theorem 2.1.3 immediately implies:

Corollary 2.1.4 *Any convex polytope P in $\mathbf{R}^d$ is a compact set.*

In the following proposition we give some simple but basic facts about polytopes and its vertices. See [12, proposition 2.2]

Proposition 2.1.5 *The following statements hold:*

- (i) *Every polytope P is the convex hull of its vertices: $P \in \text{conv}(\text{ver } t(P))$,*
- (ii) *If a polytope P can be written as the convex hull of a finite point set, then the set contains all the vertices of the polytope: $P \in \text{conv}(V)$ implies that $\text{ver } t(P) \subseteq V$.*

2.2 Barycentric coordinates

One of the important concepts related to the concept of polytope, that we need in this chapter, is the notion of barycentric coordinates, which were first introduced by August Ferdinand Möbius (1790-1816) in his book the barycentric calculus [30]. These coordinates are useful for simply representing a point in a triangle as a convex combination of its vertices, and frequently occur in computer graphics, modelling geometry triangular meshes, terrain modelling and the finite element method.

For simplices, barycentric coordinates are very common tool in many computations. Basically, they are defined as follows: let $\mathbf{x}_d \in \{\mathbf{v}_0, \dots, \mathbf{v}_d\}$ be any *linearly independent* set of $d+1$ points in $\mathbf{R}^d$, the simplex T with the set of vertices $\mathbf{x}_d$ is the convex hull of $\mathbf{x}_d$, (e.g., a triangle in 2D or a tetrahedron in 3D). Let $A_i(\mathbf{x})$ be the signed volume (or area) of the simplex created with the vertex $\mathbf{v}_i$ replaced by $\mathbf{x}$.

Then the barycentric coordinate functions $\{a_i, i \in 0, \dots, d\}$ of the simplex T with respect to its vertices are uniquely defined by:

$$a_i(\mathbf{x}) \in \frac{A_i(\mathbf{x})}{\text{vol}(T)}, \quad (2.1)$$

where $\text{vol}(T)$ will mean the volume measure of T . Since $\{\mathbf{v}_0, \dots, \mathbf{v}_d\}$ are linearly independent, then each point $\mathbf{x}$ of T has a (*unique*) representation, that is $\mathbf{x} \in \sum_{i \in 0}^d a_i(\mathbf{x}) \mathbf{v}_i$ and the barycentric coordinates $a_0, \dots, a_d$ are nonnegative *affine* functions (linear polynomials) on T , see [25, p. 288]. The uniqueness of this representation allows the weights $a_i(\mathbf{x})$ to be interpreted as an alternative set of coordinates for point $\mathbf{x}$, the so-called barycentric coordinates. Note that a simplex is a special polytope given as the convex hull of $d+1$ vertices, each pair of which is joined by an edge. In our study we need to deal with polytope in higher dimension, thus we need to generalize these coordinates to any polytope in $\mathbf{R}^d$.

2.2.1 Generalized barycentric coordinates on polytopes

Since perhaps not every reader of this topic is familiar with these coordinates, we wish to give a brief overview of the basic elements of barycentric coordinates in d -dimension, see, e. g., [15, pp.132-135] for more details. For a (convex) polytope $P \subset \mathbb{R}^d$ we will use *generalized* barycentric coordinates (They are often called generalized barycentric coordinates to distinguish them from the original barycentric coordinates, which were only defined with respect to simplices.) While barycentric coordinates are unique for simplices, there are many possible solutions for polygons with more sides. In recent years, the research on barycentric coordinates has been intensified and led to a general theory and extensions to higher dimensions [16, 17, 18, 19, 20, 1]. Usual Barycentric coordinates are natural coordinates for meshes, and their generalizations over polytopes are a very common tool in many computation. They have many useful applications including parameterization [21, 22], free form deformations [23, 18] and finite elements applications [24]. From now on let $P \subset \mathbb{R}^d$ be a polytope generated from a finite subset of points in $\mathbb{R}^d$, $W = \{x_0, \dots, x_n\}$, i.e., $P = \text{conv}(W)$. Given a polytope

$P = \text{conv}(\{x_0, \dots, x_n\})$, we wish to construct one coordinate function $\lambda_i(x)$ per point x_i for all $i = 0, \dots, n$. These functions are called barycentric coordinates with respect to $\{x_0, \dots, x_n\}$ (or P) if they satisfy three properties. First, the coordinate functions are nonnegative on P ,

$$\lambda_i(x) \geq 0, \quad (2.2)$$

for all $x \in P$. Second, the functions form a partition of unity, which means that the equation

$$\sum_{i=0}^n \lambda_i(x) = 1 \quad (2.3)$$

is verified for all $x \in P$. Finally, the functions act as coordinates in that, given a value of x , by weighting each point x_i $\lambda_i(x)$ return back x , i.e.,

$$x = \sum_{i=0}^n \lambda_i(x) x_i. \quad (2.4)$$

This last property is also sometimes referred to as linear precision since the coordinate functions can reproduce linear functions. For most potential applications, it is also preferable that these coordinate functions are as smooth as possible. Constructing the barycentric coordinates of a point x with respect to some given points in a polytope P is often not a trivial task. The first result on the existence of barycentric coordinates for more general types of polytopes was due to Kalman (1961), and will be a crucial ingredient in what follows. Indeed, we have, see [26, Theorem 2]:

Theorem 2.2.1 *Let $W = \{x_0, \dots, x_n\}$ be a set of finite points of $\mathbb{R}^d$ and let the polytope $P = \text{conv}(W)$. Then there exist nonnegative real-valued continuous functions $\lambda_0, \lambda_1, \dots, \lambda_n$ defined*

on - such that

$$\mathbf{x} \in \sum_{i \in I} \lambda_i(\mathbf{x}) \mathbf{x}_i \quad \text{and} \quad \sum_{i \in I} \lambda_i(\mathbf{x}) = 1, \quad \text{for each } \mathbf{x} \in \mathcal{K}. \quad (2.5)$$

Thus, from now on, it proves useful to work with barycentric coordinates. Therefore, unless otherwise indicated, throughout the our study it is assumed that $\lambda_i(\mathbf{x}), i \in 0, \dots, n$, are the barycentric coordinates of $\mathbf{x}$ with respect to a set of finite fixed points $\{\mathbf{x}_0, \dots, \mathbf{x}_n\}$ of the polytope

$$\mathcal{K} \subseteq \text{conv}\{\mathbf{x}_0, \dots, \mathbf{x}_n\}.$$

We shall not always trouble to repeat this at each stage. Furthermore, they need not be the vertices of $\mathcal{K}$, of course, the polytope $\mathcal{K}$ may be generated by another different set of points $\{\mathbf{y}_0, \dots, \mathbf{y}_k\}$ on $\mathcal{K}$.

For completeness, we give a result and its proof which taken from [2].

Theorem 2.2.2 *Let P be a polytope in $\mathbf{R}^d$, $\{\mathbf{v}_0, \mathbf{v}_1, \dots, \mathbf{v}_m\}$ its vertices. Then there are linearly independent nonnegative real continuous functions on P ,*

$$\lambda_i \in \{0, \dots, m\}$$

defined on P such that

$$\mathbf{x} \in \sum_{i \in I} \lambda_i(\mathbf{x}) \mathbf{v}_i \quad \text{and} \quad \sum_{i \in I} \lambda_i(\mathbf{x}) = 1, \quad \text{for each } \mathbf{x} \in P. \quad (2.6)$$

Proof The existence of a set of continuous barycentric coordinates λ_i is assured by Theorem 2.2.1. So it remains to show that the functions $\lambda_i, i \in 0, \dots, m$ are linearly independent. Linear precision (2.6) shows in particular that each $\mathbf{x}$ may be represented as a convex combination of $\mathbf{v}_0, \mathbf{v}_1, \dots, \mathbf{v}_m$. Since each $\mathbf{v}_j$ is an extreme point of P , we conclude by substituting $\mathbf{x} \in \mathbf{v}_j$ in (2.6) that $\lambda_i(\mathbf{v}_j) \in \delta_{ij}$. Hence, the functions $\lambda_0, \dots, \lambda_m$ satisfy the delta function property. Now, it is easy to see that this property implies that the set of function λ_i must be linearly independent. ■

Barycentric coordinates provide a basis for linear finite elements on simplices, and generalized barycentric coordinates naturally produce a suitable basis for linear finite elements on general polytope. The underlying principle is that one triangulates the polytope into simplices and then use the standard barycentric coordinate functions of these simplices.

Now, we present a very useful tool in our study which is triangulations of a point set and the Delaunay triangulation.

The word *triangulation* usually refers to a simplicial complex, but it has multiple meanings

when we discuss *triangulation* of some geometric entity that is being triangulated. There are triangulations of point sets, polygons, polyhedra, and many other structures. Consider points in the plane (or in any Euclidean space).

Definition 2.2.3 (triangulation of a point set) Let S be a finite set of points in the plane. A triangulation of S is a simplicial complex T such that S is the set of vertices in T , and the union of all the simplices in T is the convex hull of S , that is, $\bigcup T \in \text{conv}(S)$.

Where a simplicial complex is a collection of simplices that intersect only in mutual faces. i.e., any face of a simplex from simplicial complex T is also in T and the intersection of any two simplices $\sigma_1, \sigma_2 \in T$ is either $\emptyset$ or a face of both σ_1 and σ_2 .

Definition 2.2.4 (Simplicial decomposition) A polytope can be decomposed into a simplicial complex, or union of simplices, satisfying certain properties. Given a d -dimensional polytope P , a subset of its vertices containing $(d+1)$ affinely independent points defines an d -simplex. It is possible to form a collection of subsets such that the union of the corresponding simplices is equal to P , and the intersection of any two simplices is either empty or a lower-dimensional simplex. This **simplicial decomposition** is the basis of many methods for computing the volume of a polytope, since the volume of a simplex is easily given by a formula [31]

Definition 2.2.5 (triangulation of a point set in $\mathbf{R}^d$) The definition (2.2.3) defines a triangulation of a set of points to be simplicial complex whose vertices are the points and whose union is the convex hull of the points. With no change, the definition holds in any finite dimension d , i.e., a simplex in $\mathbf{R}^d$ is a d -dimensional simplex (d -simplex), which is defined by its $(d+1)$ vertices, and a **triangulation** of a set of points in $\mathbf{R}^d$ is a simplicial decomposition of the convex hull of the point set where the vertices of the triangles are contained in the point set.

Every finite point set in $\mathbf{R}^d$ has a triangulation see[14, 2.1]; for example, the lexicographic triangulation of [14, section 2.1] also generalizes to higher dimensions with no change.

Let S be a set of n points in $\mathbf{R}^d$. As we know from [14, section 2.1] that if all the points in S are collinear, they have one triangulation having n vertices and $n-1$ collinear edges connecting them. This is true regardless of d ; the triangulation is one-dimensional, although it is embedded in $\mathbf{R}^d$. More generally, if the affine hull of S is k -dimensional, then every triangulation of S is a k -dimensional triangulation embedded in $\mathbf{R}^d$: the simplicial complex has at least one k -simplex but no $(k+1)$ -simplex. The *complexity* of triangulation is its total number of simplices of all dimensions.

One of the famous and optimal triangulation is the *Delaunay triangulation* which is a geometric structure that engineers have used for meshes since mesh generation was in its infancy.

The *Delaunay triangulation* of a point set S , introduced by Boris Nikolavich Delaunay in 1934, is characterized by the *empty circumdisk property*: no point in S lies in the interior of any triangle's circumscribing disk; see [14, definition 1.17].

Delaunay triangulations can be generalized easily to higher dimensions ($\mathbf{R}^d$). Let S be a finite set of points in $\mathbf{R}^d$, for $d \geq 1$. Let $\triangle_k$ be a k -simplex (for any $k \leq d$) whose vertices are in S . The simplex $\triangle_k$ is Delaunay if there exists an open circumball of $\triangle_k$ that contains no point in S . Clearly, every face of a Delaunay simplex is Delaunay too.

Definition 2.2.6 (The Delaunay triangulation in $\mathbf{R}^d$) Let S be a finite point set in $\mathbf{R}^d$, and let k be the dimension of its affine hull. A Delaunay triangulation of S $Del(S)$ is a triangulation of S in which every k -simplex is Delaunay and therefore, every simplex is Delaunay. i.e., the Delaunay triangulation of a set of points in $\mathbf{R}^d$ is defined to be the triangulation such that the circumsphere of every triangle in the triangulation contains no point from the set in its interior.

Also we can present the last definition with more easy way as following:

Let $S \subseteq \mathbf{R}^d$ be a finite set of points. A Delaunay triangulation of S is a triangulation, denoted $Del(S)$, such that for each simplex $\triangle_k \in Del(S)$ there is an open d -ball that has the vertices of $\triangle_k$ on its boundary and which contains no elements of S .

Such a triangulation exists for every point set in $\mathbf{R}^d$ see [14, section 2.2], and it is the dual of the Voronoi diagram [29] (which demonstrate later). The triangulation is unique if the points are in general position.

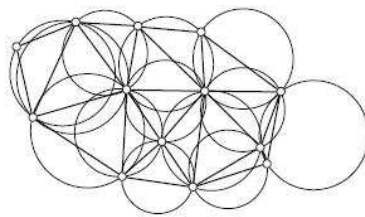


Figure 2.4 – **Every triangle in a Delaunay triangulation has an empty open circumdisk.**

The Delaunay triangulation of S is unique if and only if no four points in S lie on a common empty circle, a fact proved in [14, Section 2.7]. Otherwise, there are Delaunay triangles and edges whose interiors intersect as illustrated in the following figure.

Perhaps the most important result concerning Delaunay triangulation is the *Delaunay lemma* which proved by Boris Delaunay himself. It provides an alternative characterization of the Delaunay triangulation: a triangulation whose edges are *locally Delaunay*.

Many properties of planar Delaunay triangulation generalize to higher dimensions. A few of them are summarized below.

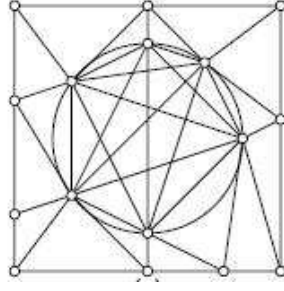


Figure 2.5 – **Delaunay triangles and edges whose interiors intersect.**

The forthcoming Delaunay lemma provides an alternative definition of a Delaunay triangulation : a triangulation of a point set in which every facet is locally Delaunay. A facet f in a triangulation T is said to be *locally Delaunay* if it is a facet of fewer than two d -simplices in T , or it is a face of exactly two d -simplices ζ_1 and ζ_2 and it has an open circumball that contains no vertex of ζ_1 nor ζ_2 . Equivalently, the open circumball of ζ_1 contains no vertex of ζ_2 . Equivalently, the open circumball of ζ_2 contains no vertex of ζ_1 . The proofs of the following lemma are omitted, but each of them is a straightforward extension of the corresponding proof for two dimension. See [14, Lemma 2.3]

Lemma 2.2.7 (Delaunay Lemma) *Let T be a triangulation of a finite d -dimensional set S of points in $\mathbf{R}^d$. The following three statements are equivalent.*

- *Every d -simplex in T is Delaunay (i.e. T is Delaunay).*
- *Every facet in T is Delaunay.*
- *Every facet in T is locally Delaunay.*

The **Voronoi diagram** is easy to describe and, via a duality relationship, it facilitates the description of the Delaunay triangulation. Given a set P of n points in $\mathbf{R}^d$, the Voronoi diagram partitions $\mathbf{R}^d$ into n cells: one cell is associated with each point in P . For $p \in P$, we denote the associated Voronoi cell by $V(p)$. The extent of $V(p)$ is simply the entire region of $\mathbf{R}^d$ whose distance to P is realized by the distance to p . That is, the set of points that is at least as close to p as it is to any other $q \in P$. Formally, we have:

Definition 2.2.8 (Voronoi diagram) *The Voronoi cell of $p \in P$ is defined by*

$$V(p) \in \{x \in \mathbf{R}^d \mid d_{\mathbf{R}^d}(p, x) \leq d_{\mathbf{R}^d}(q, x), \forall q \in P\},$$

where $d_{\mathbf{R}^d}(p, q)$ denotes the Euclidean distance between p and q in $\mathbf{R}^d$. The set of Voronoi cells forms a covering of $\mathbf{R}^d$ called the Voronoi diagram of P .

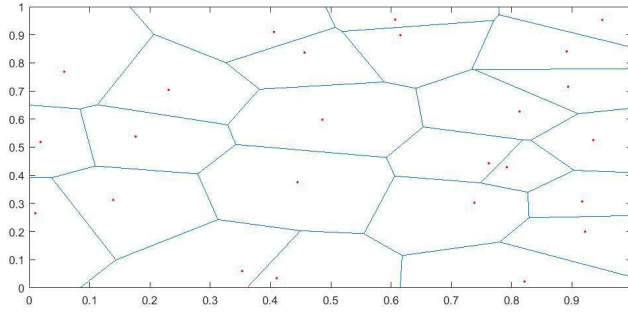


Figure 2.6 – Voronoi diagram.

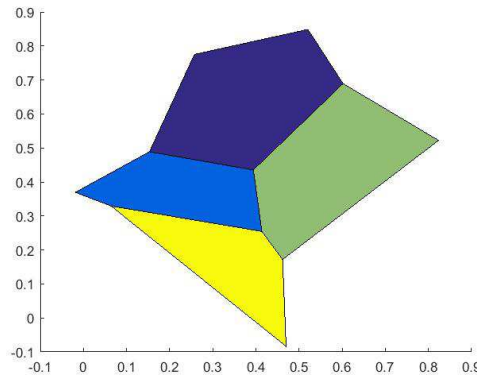


Figure 2.7 – Voronoi diagram.

2.3 Approximations of differentiable convex functions on arbitrary convex polytopes

In this section we try to approximate any arbitrary differentiable convex function on arbitrary convex polytope by using barycentric approximation. Let $X_n := \{x_i\}_{i \in \mathbb{N}}$ be a given set of $(n + 1)$ pairwise distinct points in $\mathbf{R}^d$ (called nodes or sample points), let $P \in \text{conv}(X_n)$, let f be a *convex* function with *Lipschitz continuous* gradient on P and $\lambda := \{\lambda_i\}_{i \in \mathbb{N}}$ be a set of barycentric coordinates with respect to the point set X_n . We will use the operator B_n which defined by

$$B_n[f](x) \in \sum_{i \in \mathbb{N}} \lambda_i(x) f(x_i), \quad (x \in P),$$

to approximate a convex function f which was given and analyze the error estimate between f and its barycentric approximation. Moreover, we present the best possible pointwise error estimates of f . To confirm and understand many essential and necessary steps, we starting by studying the one-dimensional case since its simplicity allows us to analyse all the necessary steps through very simple computation. In the univariate approximation, say on an interval

$[a, b]$, a simple way of approximating a given real function $f: [a, b] \rightarrow \mathbf{R}$ is to choose a partition $P := \{x_0, x_1, \dots, x_n\}$ of the interval $[a, b]$, such that $a = x_0 < x_1 < \dots < x_n = b$, and then to fit to f using a spline S_n of degree 1 at these points in such a way that:

1. The domain of S_n is the interval $[a, b]$;
2. S_n is a linear polynomial on each subinterval $[x_i, x_{i+1}]$;
3. S_n is continuous on $[a, b]$ and S_n interpolates the data, that is, $S_n(x_i) = f(x_i)$, $i = 0, \dots, n$.

This is a convenient class of interpolants because every such interpolant can be written in a barycentric form

$$S_n(x) = \sum_{i=0}^n \lambda_i(x) f(x_i), \quad (x \in [a, b]), \quad (2.7)$$

where

$$\lambda_i(x) = \begin{cases} \frac{x_{i+1} - x}{x_{i+1} - x_i}, & \text{if } x_i < x < x_{i+1}; \\ \frac{x - x_{i-1}}{x_i - x_{i-1}}, & \text{if } x_{i-1} < x < x_i; \\ 0, & \text{for all other } x. \end{cases}$$

Here, by a little abuse of notation, we set $x_{-1} := a$ and $x_{n+1} := b$. One of the main features of the usual linear spline approximation, in its simplest form (2.7), is that $\{\lambda_i\}_{i=0}^n$ form a (unique) set of (continuous) barycentric coordinates. This means that they satisfy, for all $x \in [a, b]$, three important properties:

$$\begin{aligned} \lambda_i(x) &\geq 0, \quad i = 0, \dots, n; \\ \sum_{i=0}^n \lambda_i(x) &= 1; \end{aligned}$$

$$P \subseteq \mathbf{R}^d$$

This simple approach can be generalized to general polytopes. Indeed, consider a given finite set of pairwise distinct points $X_n \subseteq \{\mathbf{x}_i\}_{i=0}^n$ in $P \subseteq \mathbf{R}^d$, with $P \subseteq \text{conv}(X_n)$ denoting the convex hull of the point set X_n . We are interested in approximating an unknown scalar-valued continuous convex function $f: P \rightarrow \mathbf{R}$ from given function values $f(\mathbf{x}_0), \dots, f(\mathbf{x}_n)$ sampled at X_n . In order to get a simple and stable global approximation of f on P , we may take into consideration a weighted average of the function values at data points of the following form:

$$B_n[f](\mathbf{x}) = \sum_{i=0}^n \lambda_i(\mathbf{x}) f(\mathbf{x}_i), \quad (2.8)$$

or, equivalently, a convex combination of the data values $f(\mathbf{x}_0), \dots, f(\mathbf{x}_n)$. This means that we require that the system of functions $\{\lambda_i\}_{i=0}^n$ forms a partition of unity, that is, for all $\mathbf{x} \in P$,

2.3. Approximations of differentiable convex functions on arbitrary convex polytopes

we have

$$n, i(\mathbf{x}) \geq 0, i \in 0, \dots, n, \quad (2.9)$$

$$\sum_{i \in 0} n, i(\mathbf{x}) = 1. \quad (2.10)$$

In view of these properties, we shall refer to the approximation schemes B_n as barycentric approximation (schemes). It should be mentioned that one of the main difficulties in obtaining *all* barycentric approximations of functions, in dimensions higher than one, lies in the fact that their construction still remains a very difficult task in the general case. However, it should be emphasized, that as in the univariate case, one possible natural approach to construct an interesting class of particular barycentric coordinates would be to simply construct a triangulation of the polytope P - the convex hull of the data set X_n - into simplices such that the vertices $\mathbf{v}_i$ of the triangulation coincide with $\mathbf{x}_i$. After that, one can use the standard barycentric coordinates for these simplices. As a result, each triangulation of the data set X_n generates a set of barycentric coordinates. Hence, there exists at least one barycentric approximation of type (2.8) which is generated by a triangulation. Let us summary shortly how triangulations and barycentric approximations are connected. It is known that every polytope can be triangulated into simplices, and the triangulation of a polytope may not be unique. To better illustrate this phenomenon, let us consider the simple example of a two-dimensional square S . Then two different triangulations are possible for S . Now every convex combination of the two associated coordinates provides a set of barycentric coordinates. This allows us to generate new families of barycentric approximations which are *not* generated by a triangulation. We refer to reference [1] for details.

A difficulty in minimizing the error estimate using the barycentric approximations arises from the possible existence of many barycentric coordinates. This yields the problem of selecting the barycentric coordinates as to minimize the approximation error. It will be interesting to have a way of selecting favourable ones among all barycentric approximations associated with the data set X_n .

Convex functions appear naturally in many specialties of science such as physics, biology, medicine and economics, and they comprise an important part of mathematics. A natural and important question is: can these functions be well approximated by simpler functions and how?

Several research discussing various methods to approximate arbitrary function, but very few ones has been done subject to the usual convexity. For instance, if some smoothness is allowed for the function f which is to be approximated, say $C^2(P)$, this will play a crucial role in the determination of the "best" (or "optimal") cubature formulas, see [1, 2, 3, 4, 5, 6, 7, 8, 9, 10].

An important part of this study is finding a barycentric approximation $B_n[f]$ of the form (2.8), which approximates f well at the points $\mathbf{x} \in P$, distinct from the data, given that f is a convex function with a Lipschitz continuous gradient. Error bounds and quality measures are provided, which estimate the influence of the barycentric coordinates on accuracy of the

approximants B_n .

When defining the set of barycentric approximants, there are two main issues to be considered. These issues are very natural and also necessary for an approximation of a given convex function f defined on an arbitrary convex polytope:

1. Since a barycentric approximation is not unique in general, it is of great interest to have a general method of constructing possible barycentric coordinates, in hope of finding the "best" barycentric approximation for a given convex function.
2. The resultant approximant, generated by this method, should not be "complicated" to implement numerically.

Our contribution in this study consists mainly of the following aspects. Firstly, under the assumption of convexity and the standard Lipschitz continuity of the gradient, we prove some results that pertain to sharp estimates of the error arising from such approximations. The most important property of barycentric approximations is that they fit into the framework of operators, since they approximate *any* convex function from above. Indeed, let $f: P \rightarrow \mathbb{R}$ be a convex function. Then, for all $x \in P$, the Jensen's inequality implies

$$f(x) \leq B_n[f](x).$$

Hence, secondly, our results also provide new upper bounds for the Jensen's inequality on an arbitrary polytope.

We knew from the previous chapter by theorem 1.3.7(4), we have that if $f \in C^{1,1}(P)$ with $L \in \mathbb{R}$ and, in addition, f be convex. Then rf satisfies the following property:

$$\frac{1}{2} \|rf(y) - rf(x)\|^2 \leq \|rf(y) - rf(x)\| \|y - x\|, \quad \forall x, y \in P, \quad (2.11)$$

where $C^{1,1}(P)$ denote the subclass of all functions f which are continuously differentiable on P with Lipschitz continuous gradients, i.e., there exists a constant L , which cannot be replaced by smaller one, such that

$$\|rf(x) - rf(y)\| \leq L \|x - y\|, \quad (\forall x, y \in P).$$

The Lipschitz continuity of rf will play a crucial role in our analysis. This lead to the following result which taken from [32, see proposition 2.2].

Proposition 2.3.1 *If $f \in C^{1,1}(P)$ with Lipschitz constant $L \in \mathbb{R}$, then the functions defined by*

$$g_\lambda := \frac{L}{f} \|f\|_k^2$$

2.3. Approximations of differentiable convex functions on arbitrary convex polytopes

are both convex and belong to $C^{1,1}(P)$. If in addition f is convex, then $L_{g_i} \leq L_f$.

Proof The proof is similar to that in [32], but here we give more details.

We need to show that the functions $g_\S$ also belong to $C^{1,1}(P)$. Indeed, they are obviously differentiable and it is easy to check that

$$\| \nabla g_\S(y) - \nabla g_\S(x) \| \leq L \| \nabla f(y) - \nabla f(x) \| \quad (2.12)$$

which implies, using the triangle inequality,

$$\begin{aligned} \| \nabla g_\S(y) - \nabla g_\S(x) \| &\leq L \| \nabla f(y) - \nabla f(x) \| \\ &\leq 2L \| \nabla f(y) - \nabla f(x) \|. \end{aligned}$$

Hence, we have $L_{g_\S} \leq 2L_f$. Moreover, since $f \in C^{1,1}(P)$, then by the Cauchy-Schwartz inequality we have

$$\begin{aligned} \langle \nabla f(y) - \nabla f(x), y - x \rangle &= \langle \nabla f(y) - \nabla f(x), y - x \rangle \leq \| \nabla f(y) - \nabla f(x) \| \| y - x \| \\ &\leq L_f \| y - x \|^2 \end{aligned}$$

then,

$$\langle \nabla g_\S(y) - \nabla g_\S(x), y - x \rangle \leq L_f \| y - x \|^2 \quad (2.13)$$

and so

$$L_f \| y - x \|^2 \geq \langle \nabla g_\S(y) - \nabla g_\S(x), y - x \rangle \geq 0. \quad (2.14)$$

From this, it immediately follows

$$\langle \nabla g_\S(y) - \nabla g_\S(x), y - x \rangle \leq L_f \| y - x \|^2 \geq 0,$$

which means that $g_\S$ are both convex.

What remains to be shown is that if f is in addition convex, we have $L_{g_i} \leq L_f$. Since function g_i has a Lipschitz continuous gradient, then from the convexity of f together with equation

2.11, it follows

$$\begin{aligned} |g_i(y) - g_i(x)| &\leq L_{g_i} \|y - x\| \\ &\leq L_{g_i} \|y - x\| + L_f \|y - x\| \\ &\leq (L_{g_i} + L_f) \|y - x\| \end{aligned}$$

then,

$$\begin{aligned} \|g_i(y) - g_i(x)\| &\leq \frac{L_{g_i} + L_f}{q} \|y - x\| \\ L_{g_i} \|y - x\| &\leq \frac{L_{g_i} + L_f}{q} \|y - x\| \end{aligned}$$

This allows us to conclude that $L_{g_i} \leq L_f$, since L_{g_i} is the smallest possible Lipschitz constant. This completes the proof of Proposition 2.3.1. ■

We are now in a position to state and prove our announced simple and elegant characterization of all upper approximation operators. For completeness, we now give another result and its proof from [32, see Theorem 2.3].

Theorem 2.3.2 Let $A : C^1(P) \rightarrow C(P)$ be a linear operator. The following statements are equivalent:

(i) For every convex function $g \in C^{1,1}(P)$, we have

$$g(x) = A[g](x), \quad (x \in P). \quad (2.15)$$

(ii) For every $f \in C^{1,1}(P)$ with a Lipschitz constant L_f , we have

$$|f(x) - A[f](x)| \leq \frac{L_f}{2} \|A[k, k^2](x) - kx\|^2. \quad (2.16)$$

Equality is attained for all functions of the form

$$f(x) = a(x) + c\|x\|^2, \quad (2.17)$$

where $c \in \mathbb{R}$ and $a(\cdot)$ is any affine function.

2.3. Approximations of differentiable convex functions on arbitrary convex polytopes

Proof The proof is similar to that in [32], but we give more details.

Let $f \in C^{1,1}(P)$ with a Lipschitz constant L_f and suppose that (i) holds. Define the two following functions

$$g \in \mathcal{A} : \mathcal{A} \left(\frac{L_f}{2} \|k\|^2 \right) \leq f$$

Due to proposition 2.3.1, we know that both of these functions are convex and belong to $C^{1,1}(P)$. Therefore, since A is linear, statement (i) implies that

$$\begin{aligned} A \left(\frac{L_f}{2} \|k\|^2 \right) \leq f &\leq \frac{L_f}{2} \|k\|^2 \leq f \\ A \left(\frac{L_f}{2} \|k\|^2 \right) \leq A f &\leq \frac{L_f}{2} \|k\|^2 \leq f \end{aligned}$$

$$\frac{L_f}{2} A[\|k\|^2] \leq A[f] \leq \frac{L_f}{2} \|k\|^2 \leq f,$$

which gives the error estimate in statement (ii). The case of equality is easily verified.

Conversely, let $g \in C^{1,1}(P)$ be a convex function, and suppose that statement (ii) holds. Let the function f be defined by

$$f \in \mathcal{A} : \mathcal{A} \left(\frac{L_g}{g} \|k\|^2 \right) \leq g$$

and set $E \in \mathcal{A} : E \leq I$, where I is the identity on $C^{1,1}(P)$. Applying proposition 2.3.1 again, we have $f \in C^{1,1}(P)$ with $L_f \leq L_g$. Now, the error estimate in statement (ii), applied to f , implies that

$$\begin{aligned} E \left(\frac{L_g}{2} \|k\|^2 \right) \leq g &\leq \frac{L_f}{2} E[\|k\|^2] \\ &\leq \frac{L_g}{2} E[\|k\|^2] \end{aligned}$$

$$\frac{L_g}{2} E[\|k\|^2] \leq E[g] \leq \frac{L_g}{2} E[\|k\|^2]$$

This shows that $E[g] = 0$, as was to be proved. ■

Note that in the error estimate established in Theorem 2.3.2 below, it is not required that the function f be convex as long as statement (i) holds. The latter condition, as mentioned previously, is always satisfied by our barycentric approximation operator B_n . Hence, Jensen's inequality and Theorem 2.3.2 imply the following error estimate see [32, Corollary 2.4].

Corollary 2.3.3 *Let B_n be the barycentric approximation given by (2.8). Then for every function $f \in C^{1,1}(P)$ with a Lipschitz constant L_f , we have*

$$\|f(x) - B_n[f](x)\| \leq \frac{L_f}{2} \|B_n[k, k^2](x) - kx\|^2. \quad (2.18)$$

Equality is attained for all functions of the form (2.17).



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3 On the approximation of strongly convex functions by an upper or lower operator

This chapter is based on our paper [14], however, here, we choose to give new proofs of our main results, based on completely different technique such as some simple characterizations of positive linear operators in the set of convex functions, see Lemma 3.1.1. The aim of this chapter is to find a convenient and practical method to approximate a given real-valued function of multiple variables by linear operators, which approximate all *strongly* convex functions from above (or from below). Our main contribution is to use this additional knowledge to derive sharp error estimates for continuously differentiable functions with Lipschitz continuous gradients. More precisely, we show that the error estimates based on such operators are always controlled by the Lipschitz constants of the gradients and the error associated with using the quadratic function, see Theorems 3.2.1 and 3.2.3. Moreover, assuming the function, we want to approximate, is also strongly convex, we establish sharp upper as well as lower refined bounds for the error estimates, see Corollaries 3.2.2 and 3.2.4. As an application, we define and study a class of linear operators on an arbitrary polytope, which approximate strongly convex functions from above. Finally, we present a numerical example illustrating the proposed method.

3.1 Some background and motivation

Let $C \subset \mathbb{R}^d$ be a nonempty compact convex set and let $f : C \rightarrow \mathbb{R}$ be a given function. We would like to find an easier and good approximation to compute f . We sometimes know beforehand that the function f satisfies various known structural and regularity properties. For example, it may be known that f has some additional kind of convexity, therefore we would wish to use this information in order to get a good approximation of f . Approximating an arbitrary function is, in general, very difficult, but if we restrict our attention to the class of strongly convex functions and if the linear operator, we wish to use, approximates all *strongly* convex functions from above (or from below) then things become simpler. The strongly convex

functions are used widely in economic theory (see [1]), and are also central to optimization theory (see [2]). Indeed, in the framework of function minimization, this convexity notion has important and well-known implications. As we will see, the key advantage of dealing with such an operator is that an estimate of its approximation error is always controlled by the error associated with using the quadratic function.

In order to illustrate this idea more precise, we start by describing briefly a specific one-dimensional example, since its simplicity allows us to analyze all the necessary steps through very simple computation. Suppose that τ is a fixed nonnegative real number. In the univariate approximation, say on an interval $[a, b]$, a simple way of approximating a given real τ -strongly convex function $\hat{A} : [a, b] \rightarrow \mathbf{R}$ is first to choose a partition $P : \mathcal{A} \{x_0, x_1, \dots, x_n\}$ of the interval $[a, b]$, such that $a \in x_0 \leq x_1 \leq \dots \leq x_n \in b$, and then to fit to $\hat{A}$ using a linear interpolant B_n at these points in such a way that:

1. The domain of B_n is the interval $[a, b]$;
2. B_n is a linear polynomial on each subinterval $[x_i, x_{i+1}]$;
3. B_n is continuous on $[a, b]$ and it interpolates the data, that is, $B_n(x_i) \in \hat{A}(x_i)$, $i \in 0, \dots, n$.

This is a convenient class of interpolants because every such interpolant can often be written for all $i \in 0, \dots, n-1$ in a barycentric form:

$$B_n[\hat{A}](x) \in \frac{x_{i+1} - x}{x_{i+1} - x_i} \hat{A}(x_i) + \frac{x - x_i}{x_{i+1} - x_i} \hat{A}(x_{i+1}), \quad (x \in [x_i, x_{i+1}]). \quad (3.1)$$

One of the main features of the usual linear interpolant, in its simplest form (3.1), is that the error in approximating the quadratic function $(\cdot)^2$ by B_n is simply given by:

$$B_n[(\cdot)^2](x) - x^2 \in (x - x_i)(x_{i+1} - x), \quad (x \in [x_i, x_{i+1}]),$$

and also that B_n approximates all τ -strongly convex functions from above. More precisely, B_n satisfies for any τ -strongly convex function the following estimates:

$$\frac{1}{2}(x - x_i)(x_{i+1} - x) \cdot B_n[f](x) - f(x), \quad (x \in [x_i, x_{i+1}]).$$

Moreover, as it can be derived from our multivariate general results, see Remark 3.3.5, if we also know that the first derivative of f is a Lipschitz function with a local Lipschitz constant $L_i(f^0)$ in the subintervals $[x_i, x_{i+1}]$, then the error $B_n[f] - f$ can often be estimated at any $x \in [x_i, x_{i+1}]$ as:

$$\frac{1}{2}(x - x_i)(x_{i+1} - x) \cdot B_n[f](x) - f(x) \leq \frac{L_i(f^0)}{2}(x - x_i)(x_{i+1} - x). \quad (3.2)$$

Hence, the lower and upper bounds of the approximation error for this class of functions can be controlled by the Lipschitz constants of the first derivatives, the convexity parameter (of

the strong convexity) and the error associated with using the quadratic function. It should be noted that equalities in (3.2) are attained for all ℓ -strongly convex functions of the form

$$f(x) \in a(x) + \frac{\ell}{2}x^2, \quad (3.3)$$

where $a(\cdot)$ is any affine function. Therefore, in this sense, the error estimates (3.2) are sharp for the class of ℓ -strongly convex functions having Lipschitz continuous first derivatives. This provides the starting point of the forthcoming results.

This chapter deals with the problem of approximation of functions of multiple variables by using linear operators, which approximate from above (or from below) all strongly convex functions with Lipschitz-continuous gradients. Geometrically, if a function f belongs to such a class, then its gradient ∇f cannot change too quickly and it cannot change too slowly either. Functions satisfying these conditions are widely used in the optimization literature, we refer to Nesterov's book [2]. A natural question is: can these functions be well approximated by simpler functions and how?

There are several studies investigating various methods to approximate arbitrary functions, very little research has been done subject to some kind of additional convexity assumption. For instance, if some smoothness is allowed for the function, which is to be approximated, say $C^2(\cdot)$, this will play a crucial role in the determination of the "best" (or "optimal") cubature formulas, see [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. This chapter builds on the previous work [5, 6], where a theoretical framework for approximating $C^2(\cdot)$ -convex functions was developed.

The motivation for such an approach is that the general sharp error estimates, that we derive, permit us to study a multivariate version defined on an arbitrary (convex) polytope of the univariate interpolation operators given by (3.1). Throughout the chapter, a linear operator is said to be upper (resp. lower) operator for strongly convex functions, if it approximates from above (resp. from below) strongly convex functions.

For any differentiable f with Lipschitz continuous gradient, there exists a smallest possible $L(\nabla f)$ such that (1.25) holds. The smallest constant $L(\nabla f) : \in \text{Li p}(\nabla f)$ satisfying the inequality (1.25) is called the Lipschitz constant for ∇f . While the Lipschitz constant provides an upper bound for the "curvature" of the function, the convexity parameter determines a lower bound. By $C^{1,1}(\cdot)$ we will denote the subclass of all functions f which are continuously differentiable on $\cdot$ with Lipschitz continuous gradients.

The chapter is organized as follows: In Section 3.1 we give some background, motivation and state the idea more precise of approximate strongly convex function in one-dimensional case also give very important lemma see (Lemma 3.1.1). The main theorems of Section 3.2 establish, in terms of sharp error estimates, simple and elegant characterizations of upper or lower approximation operators for strongly convex functions with Lipschitz-continuous

gradients. In this way, we offer sharp error estimates which only depend on the Lipschitz constants of the gradients and the error associated with using the quadratic function, see Theorems 3.2.1 and 3.2.3. A particularly interesting situation arises, when the function, we want to approximate, is also strongly convex. In this case, we establish sharp upper as well as lower refined bounds for the error estimates, see Corollaries 3.2.2 and 3.2.4. In Section 3.3, we will introduce and study a multivariate version defined on an arbitrary polytope of the univariate interpolation operators given by (3.1). Finally, Section 3.4 will provide a numerical example to illustrate the efficiency of this approach.

In what follows, we continue to denote by $S^{\mu,1}(-)$ the set of μ -strongly convex continuously differentiable functions with Lipschitz-continuous gradients. Note that, as we have mentioned before, for any $f \in S^{\mu,1}(-)$ we always have $\mu \leq L(f)$. It is also quite easy to see that for a convex quadratic $f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T H \mathbf{x}$, the Lipschitz constant of the gradient is given by the maximal eigenvalue of the Hessian H while the parameter of strong convexity is given by its minimal eigenvalue. Hence, for any nonnegative μ , the function $\bar{f}(\mathbf{x}) = \frac{\mu}{2} \|\mathbf{x}\|^2$ defines a μ -strongly convex function with a Lipschitz gradient constant $L(\bar{f})$ equal to μ .

The following Lemma provides simple characterizations of positive linear operators in the set of convex functions. This result implies in particular that in order to prove that a linear operator $E : C(-) \rightarrow C(-)$ is positive in the set of convex functions, it suffices to verify that E is positive in a given set of strongly convex functions with a certain strong convexity parameter.

Lemma 3.1.1 *Let μ be an arbitrary fixed positive number and let $E : C(-) \rightarrow C(-)$ be a linear operator. Then the following statements are equivalent:*

(i) *For every convex function $f \in C(-)$, we have*

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

(ii) *For every μ -strongly convex function $f \in C(-)$, we have*

$$E(f) \geq \frac{\mu}{2} E(\|\cdot\|^2) \geq 0.$$

(iii) *For every μ -strongly convex function $f \in C(-)$, we have*

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

(iv) *For every $\mu \geq 0$ and every μ -strongly convex function f , we have*

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

3.2. Characterizations of upper or lower approximation operators

Proof To prove (i) implies (ii), assume that (i) holds. Let f be $\frac{1}{2}$ -strongly convex function. Set $g := f + \frac{1}{2} k \cdot k^2$. By Theorem 1.2.5, we know that g is convex. Therefore, applying property (i) we get: Hence, by linearity of E , we deduce that

$$E(f) \leq \frac{1}{2} E(k \cdot k^2).$$

Since $k \cdot k^2$ is convex, then again by (i) we have $E(k \cdot k^2) \geq 0$. This shows that (ii) holds. Now, (ii) implies (iii) is obvious. Next assume that (iii) holds. Let ϵ be a positive real number. Let f be a ϵ -strongly convex function. Then, by Theorem 1.2.5

$$g := f + \frac{\epsilon}{2} k \cdot k^2,$$

is convex. Observe that:

$$\frac{1}{\epsilon} g := \frac{1}{\epsilon} f + \frac{1}{2} k \cdot k^2.$$

Furthermore, since $\frac{1}{\epsilon} g$ is convex, then $\frac{1}{\epsilon} f$ is $\frac{1}{2}$ -strongly convex. Hence, by (iii) we can conclude that

$$E\left(\frac{1}{\epsilon} f\right) \geq 0.$$

Thus it follows that

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

This shows that (iv) holds.

Finally, assume that the property (iv) holds and take any convex function f . Since $f + \frac{\epsilon}{2} k \cdot k^2$ is ϵ -strongly convex, then by (iv), we have

$$E\left(f + \frac{\epsilon}{2} k \cdot k^2\right) \geq 0,$$

or equivalently

$$E(f) \geq -\frac{\epsilon}{2} E(k \cdot k^2).$$

In view of the fact that this inequality holds for all $\epsilon \geq 0$, then by letting $\epsilon \rightarrow 0$, it follows that

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

Hence, the four statements are equivalent. ■

3.2 Characterizations of upper or lower approximation operators

In this section, the first main results, Theorems 3.2.1 and 3.2.3 are on simple characterizations, in terms of sharp error estimates, of approximation operators, which approximate from below or above strongly convex functions with Lipschitz continuous gradients. It is shown that the error estimates using these operators can often be controlled by the Lipschitz constants of the gradients and the error associated with using the quadratic function. The second

On the approximation of strongly convex functions by an upper or lower operator

ones, which are their Corollaries 3.2.2 and 3.2.4, are on the establishment of sharp upper as well as lower refined bounds for the error estimates, assuming that the function, which is to be approximated, is also strongly convex. Here, we continue to assume that the strong convexity parameter τ is given (possibly null). Our characterization of linear operators, which approximate all τ -strongly convex functions from above, is as follows:

Theorem 3.2.1 *Let τ be a positive real number and let $A : C^{1,1}(-) \rightarrow C(-)$ be a linear operator. Then, the following two statements are equivalent:*

(i) *For every τ -strongly convex function $g \in C^{1,1}(-)$, we have*

$$g(x) \leq A g(x), \quad (x \in \mathbb{R}). \quad (3.4)$$

(ii) *For every function $f \in C^{1,1}(-)$, we have*

$$|A f(x) - f(x)| \leq \frac{L(f)}{2} \|A\|_{k,k}^2 (x) \|x\|^2, \quad (x \in \mathbb{R}). \quad (3.5)$$

Proof Assume that (i) holds and let E be the linear operator defined by

$$E f = A f - \tau f.$$

Then, by (i), we have

$$E f \geq 0,$$

for all τ -strongly convex function. By Lemma 3.1.1, we have

$$E f \geq 0,$$

for all convex function, therefore by Theorem 2.3.2 (ii) holds. Now, assume that (ii) holds. Then, by Theorem 2.3.2, we have

$$E f \geq 0$$

for all convex functions. Thus, by Lemma 3.1.1, we have

$$E f \geq 0$$

for all τ -strongly convex functions. $\blacksquare$

Theorem 3.2.1 extends a result given in [5, Theorem 2.3] for convex functions to the case of strongly convex functions.

We already know how one can estimate the approximation error $|A f - f|$ for a function possessing Lipschitz continuous gradient; what happens if we know in advance that the

3.2. Characterizations of upper or lower approximation operators

function is, moreover, strongly convex?

The answer is given by the following Corollary, which is a direct consequence of Theorem 3.2.1.

Corollary 3.2.2 *Let ℓ be a positive real number and let $A : C^1(-) \rightarrow C(-)$ be a linear operator. Assume that for every convex function $g \in C^{1,\ell}(-)$, we have*

$$A[g](x) \leq g(x), \quad (x \in \mathbb{R}). \quad (3.6)$$

Then the following error estimates hold for every ℓ -strongly convex function $f \in S^{1,\ell}(-)$:

$$\frac{1}{2} E_A[k,k](x) \cdot A[f](x) \leq f(x) \leq \frac{1}{2} E_A[k,k](x), \quad (x \in \mathbb{R}), \quad (3.7)$$

where $E_A[k,k^2] \leq A[k,k^2] \leq k \cdot k^2$. Equalities in (3.7) are attained for all functions of the form

$$f(x) \in a(x) \pm \frac{1}{2} k x^2, \quad (3.8)$$

where $a(\cdot)$ is any affine function.

Proof The error upper bound is a direct consequence of Theorem 3.2.1. So it remains to check that the error lower bound holds, too. Assume that the statement (i) holds for every convex function and let us fix a ℓ -strongly convex function f . Then, since $g \in f \pm \frac{1}{2} k \cdot k^2$ is convex, statement (i) and the linearity of A imply

$$f \leq \frac{1}{2} k \cdot k^2 \cdot A[f] \leq A[k \cdot k^2],$$

or equivalently

$$\frac{1}{2} A[k \cdot k^2] \leq k \cdot k^2 \leq A[f] \leq f.$$

This shows that $\frac{1}{2} E_A[k,k^2]$ estimates $A[f] \leq f$ from below and completes the proof of the lower bound. Finally, since A reproduces linear and constant functions, the case of equality can be confirmed by a little algebra. ■

According to the error estimates (3.5) and (3.7), Corollary 3.2.2 provides a better error lower bound than Theorem 3.2.1 for strongly convex functions with Lipschitz continuous gradients. A slight modification of Theorem 3.2.1 given below addresses the case in which the linear operator A , we wish to use, approximates all convex functions from below. Indeed, in this setting our characterization of those operators can be stated as follows:

Theorem 3.2.3 *Let ℓ be a positive real number and let $A : C^1(-) \rightarrow C(-)$ be a linear operator. The following statements are equivalent:*

(i) For every ℓ -strongly convex function $g \in C^{1,1}(\cdot)$, we have

$$A[g](\mathbf{x}) \leq g(\mathbf{x}), \quad (\mathbf{x} \in \mathbb{R}^d). \quad (3.9)$$

(ii) For every function $f \in C^{1,1}(\cdot)$, we have

$$A[f](\mathbf{x}) \leq f(\mathbf{x}) + \frac{L(f)}{2} \|\mathbf{x}\|^2, \quad (\mathbf{x} \in \mathbb{R}^d). \quad (3.10)$$

Note that in the error estimates (ii), established in Theorems 3.2.1 and 3.2.3, are valid for all functions in $C^{1,1}(\cdot)$, as long as statements (i) hold for the class of ℓ -strongly convex functions. We remark here that similar arguments to those used in Corollary 3.2.2 will derive the following refined error estimates:

Corollary 3.2.4 Let ℓ be a positive real number and let $A : C^{1,1}(\cdot) \rightarrow C(\cdot)$ be a linear operator. Assume that for every convex function $g \in C^{1,1}(\cdot)$, we have

$$A[g](\mathbf{x}) \leq g(\mathbf{x}), \quad (\mathbf{x} \in \mathbb{R}^d). \quad (3.11)$$

Then the following error estimates hold for every ℓ -strongly convex function $f \in S^{1,1}(\cdot)$:

$$\frac{1}{2} E_{\|\cdot\|^2}(\mathbf{x}) \leq f(\mathbf{x}) - A[f](\mathbf{x}) \leq \frac{L(f)}{2} E_{\|\cdot\|^2}(\mathbf{x}), \quad (\mathbf{x} \in \mathbb{R}^d), \quad (3.12)$$

where $E_{\|\cdot\|^2}(\mathbf{x}) = \|\mathbf{x}\|^2 - A[\|\cdot\|^2](\mathbf{x})$. Equalities in (3.12) are attained for all functions of the form

$$f(\mathbf{x}) \in a(\mathbf{x}) + \frac{1}{2} \|\mathbf{x}\|^2, \quad (3.13)$$

where $a(\cdot)$ is any affine function.

3.3 Applications to the barycentric approximation schemes

In this section, we are going to consider a multivariate version different from the tensor product construction that in the univariate case, $d \in \mathbb{N}$, yields the operator defined by (3.1). Indeed, the simple univariate operator (3.1) can be extended to arbitrary higher-dimensional polytopes. To this end, let $X_n \in \{\mathbf{x}_i\}_{i \in \mathbb{N}}$ be a given finite set of pairwise distinct points in

$\frac{1}{2} \mathbf{R}^d$, with $\cdot \in \text{conv}(X_n)$ denoting the convex hull of the point set X_n . We are interested in approximating an unknown scalar-valued continuous ℓ -strongly convex function $f : \cdot \rightarrow \mathbf{R}$

from given function values $f(\mathbf{x}_0), \dots, f(\mathbf{x}_n)$ sampled at X_n . In order to obtain a simple and stable global approximation of f on $\cdot$, we may consider a weighted average of the function values at data points of the following form:

$$B_n[f](\mathbf{x}) \in \sum_{i \in \mathbb{N}} \lambda_i(\mathbf{x}) f(\mathbf{x}_i), \quad (3.14)$$

3.3. Applications to the barycentric approximation schemes

or, equivalently, a convex combination of the data values $f(\mathbf{x}_0), \dots, f(\mathbf{x}_n)$. This means that we require the system of functions $\{j_i : \mathbf{x} \in \mathbb{R}^2\}_{i=0}^n$ to form a partition of unity, that is, for all $\mathbf{x} \in \mathbb{R}^2$, we have

$$j_i(\mathbf{x}) \geq 0, \quad i = 0, \dots, n, \quad (3.15)$$

$$\sum_{i=0}^n j_i(\mathbf{x}) = 1. \quad (3.16)$$

In addition, we shall also impose the set of functions j_i to satisfy the first-order consistency condition:

$$\mathbf{x} \in \mathbb{R}^2 \implies \sum_{i=0}^n j_i(\mathbf{x}) \mathbf{x}_i = \mathbf{x}. \quad (3.17)$$

We will call any set of functions $j_i : \mathbb{R}^2 \rightarrow \mathbb{R}$, $i = 0, \dots, n$, *barycentric coordinates* if they satisfy the three properties (3.15), (3.16) and (3.17) for all $\mathbf{x} \in \mathbb{R}^2$. In view of these properties, we shall refer to the approximation schemes B_n as barycentric approximation (schemes). Recall that these coordinates exist for more general types of polytopes. The first result on their existence was due to Kalman [13, Theorem 2] (1961). Let us go back now to the simple case of a univariate function f for the computation of a barycentric approximation function created in this manner. To do this, we consider a subinterval $[x_i, x_{i+1}]$, then it is easily seen that the barycentric coordinates of a point x of $[x_i, x_{i+1}]$ with respect to $v_0 \in [x_i, x_{i+1}]$, $v_1 \in [x_i, x_{i+1}]$ are given respectively as follows:

$$j_{i,0}(x) = \frac{x_{i+1} - x}{x_{i+1} - x_i},$$

$$j_{i,1}(x) = \frac{x - x_i}{x_{i+1} - x_i}.$$

This shows that in one dimension the barycentric approximation function (3.14) is nicely reduced to the simple form given in (3.1). Hence, our proposed method of approximation scheme (3.14) can be viewed as a multivariate generalization of the approach in the univariate case.

For a τ -strongly convex function $f \in S^{\tau,1}(\cdot)$, the symbol

$$E_n[f](\mathbf{x}) := E_n[f, j_i](\mathbf{x}) = \sum_{i=0}^n j_i(\mathbf{x}) f(\mathbf{x}_i) - f(\mathbf{x}), \quad (\mathbf{x} \in \mathbb{R}^2), \quad (3.18)$$

will be reserved exclusively to denote the incurred approximation error between f and its barycentric approximation $B_n[f]$.

We begin our analysis by giving general identities, which show simple expressions of the error

3.3. Applications to the barycentric approximation schemes

Equality in (3.21) is attained for all functions of the form

$$f(\mathbf{x}) \in a(\mathbf{x}) \pm \frac{1}{2} \|\mathbf{x}\|^2, \quad (3.22)$$

where $a(\cdot)$ is any affine function.

Proof Let us fix f a $\frac{1}{2}$ -strongly convex function and define $h := f + \frac{1}{2} \|\cdot\|^2$. Since, h is convex then by the Jensen-convexity of h , we get

$$h(\mathbf{x}) \leq \sum_{i \in \mathcal{I}} \lambda_i h(\mathbf{x}_i), \quad (\mathbf{x} \in \mathcal{C}).$$

Or equivalently

$$f(\mathbf{x}) + \frac{1}{2} \|\mathbf{x}\|^2 \leq \sum_{i \in \mathcal{I}} \lambda_i \left(f(\mathbf{x}_i) + \frac{1}{2} \|\mathbf{x}_i\|^2 \right), \quad (\mathbf{x} \in \mathcal{C}).$$

Thus, we get

$$\frac{1}{2} \|\mathbf{x}\|^2 \leq \sum_{i \in \mathcal{I}} \lambda_i \left(\frac{1}{2} \|\mathbf{x}_i\|^2 \right) + f(\mathbf{x}) - \sum_{i \in \mathcal{I}} \lambda_i f(\mathbf{x}_i) = f(\mathbf{x}) - B_n[f](\mathbf{x}).$$

This inequality, combined with Lemma 3.3.1, implies that the required identity is satisfied. The case of equality is easily verified. ■

The following Lemma gives an upper bound for the absolute value of the error of any function possessing Lipschitz continuous gradient:

Lemma 3.3.3 The following error estimate holds for every function $f \in C^{1,1}(\cdot)$:

$$|B_n[f](\mathbf{x}) - f(\mathbf{x})| \leq \frac{L(f)}{2} \sum_{i \in \mathcal{I}} \lambda_i \|\mathbf{x} - \mathbf{x}_i\|^2, \quad (\mathbf{x} \in \mathcal{C}). \quad (3.23)$$

Equality in (3.23) is attained for all functions of the form

$$f(\mathbf{x}) \in a(\mathbf{x}) \pm \frac{1}{2} \|\mathbf{x}\|^2, \quad (3.24)$$

where $a(\cdot)$ is any affine function.

Proof This Lemma is an immediate consequence of Corollary 3.2.4 and Lemma 3.3.1. The case of equality is easily verified. ■

Now everything is set for giving an upper bound and a lower bound for the error estimate $B_n[f] - f$ of any $\frac{1}{2}$ -strongly convex function f , having Lipschitz continuous gradient.

Theorem 3.3.4 Let τ be a positive real number. Then, for every τ -strongly convex function $f \in S^{1,1}(\cdot)$ and any $\mathbf{x} \in \mathbb{R}^n$, it holds:

$$\frac{\tau^n}{2} \|\mathbf{x}\|^2 \leq \sum_{i \in \mathcal{I}} \lambda_i(\mathbf{x}) \|\mathbf{x} - \mathbf{x}_i\|^2 \leq B_n[f](\mathbf{x}) - f(\mathbf{x}) \leq \frac{L(f)}{2} \sum_{i \in \mathcal{I}} \lambda_i(\mathbf{x}) \|\mathbf{x} - \mathbf{x}_i\|^2. \quad (3.25)$$

Equality in (3.25) is attained for all functions of the form

$$f(\mathbf{x}) \in a(\mathbf{x}) + \frac{\tau}{2} \|\mathbf{x}\|^2, \quad (3.26)$$

where $a(\cdot)$ is any affine function.

Proof This is an immediate consequence of Lemmas 3.3.2, 3.3.3 and Corollary 3.2.4. The case of equality is easily verified. ■

Remark 3.3.5 In the univariate case, a simple inspection of the error estimates (3.25) reveals that (3.25) is nicely reduced to the simple form given in (3.2).

3.4 Numerical experiments

One possible natural approach to construct an interesting class of particular barycentric approximations would be to simply construct a triangulation of the polytope $\mathcal{K}$ - the convex hull of the data set $X_n \in \{\mathbf{x}_i\}_{i \in \mathcal{I}}$ - into simplices such that the vertices $\mathbf{v}_j$ of the triangulation coincide with the data points $\mathbf{x}_j$. After that, one can use the standard barycentric coordinates for these simplices. As a result, each triangulation of the data set X_n generates a barycentric approximation. Hence, there exists at least one barycentric approximation of type (3.14) which is generated by a triangulation. A very natural triangulation $DT(\cdot)$ of $\mathcal{K}$ is the one which uses only the points of X_n as triangulation vertices and such that no point in X_n lies *inside* the circumscribing ball of any simplex of $DT(\cdot)$. Such a triangulation exists and is called a Delaunay triangulation of $\mathcal{K}$ with respect to X_n .

Let $T(\cdot)$ be any triangulation of the point set X_n . Then $\lambda_i^T(\cdot) \in \mathbb{R}^n$ denotes the set of barycentric coordinates associated with each $\mathbf{x}_i$ of X_n . We now list the basic properties of $\lambda_i^T(\cdot)$ of which the following are particularly relevant to us:

- (1) They are well-defined, piecewise linear and nonnegative real-valued continuous functions.
- (2) The function $\lambda_i^T(\cdot)$ has to equal 1 at $\mathbf{x}_i$ and 0 at all other points in $X_n \setminus \{\mathbf{x}_i\}$, that is, $\lambda_i^T(\mathbf{x}_j) \in \delta_{ij}$ (δ is the Kronecker delta).

We denote by

$$E_n^{T(-)}[f](\mathbf{x}) := \sum_{i \in \mathcal{N}} T_i^{(-)}(\mathbf{x}) f(\mathbf{x}_i) \approx f(\mathbf{x}).$$

As regard the error estimates (3.25), it was shown that Delaunay triangulation is the triangulation that minimizes the approximation error $E_n^{T(-)}[f](\mathbf{x})$ among all triangulations with the same number of vertices, see [5, Theorem 4.10]. This optimality condition also characterizes Delaunay triangulation.

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Suppose a set of scattered data $(x_i, y_i, f_i) \ i \in \mathcal{N}$, which are assumed to be sampled from a strongly convex function $f : \mathbb{R}^2 \rightarrow \mathbb{R}$. Taking the N scattered points as nodes, a barycentric approximation is constructed in domain D using Delaunay triangulation. We now illustrate this approach by the following numerical example:

Example 3.4.1 We take the following strongly convex function:

$$f(x, y) := 100((x - 0.4)^2 + (y - 0.5)^2) + 400 \exp((x - 0.5)^2 + (y - 0.5)^2),$$

with the restriction of domain $D := [0, 1] \times [0, 1]$. The data is generated from the above function and it is based on 21 equally spaced nodes on each edge of the boundary of square D and 216 nodes in the square D . The nodes in the domain are placed randomly selected from D while the nodes on the boundary is equally spaced. From Figure 3.1 it is clear that the strong convexity of f has been preserved and there is no visual difference between the test function and its piecewise-linear interpolant.

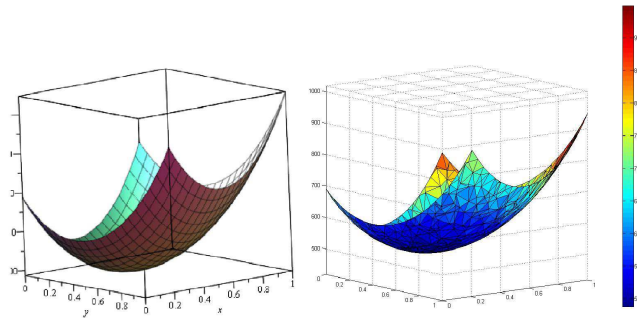


Figure 3.1 – The figure on the left shows the graph of f produced by MAPLE, and using MAT-LAB the graph on the right is for the piecewise-linear interpolation of the data generated from f .

3.5 Numerical examples and MSE error

In order to give numerical illustrations of the performance of our implementation of barycentric approximation, we apply the method to the reconstruction of four test functions $f_k, k \in 1, \dots, 4$, when the domain Ω is a square or a cube, and the function f_k exhibits the following features: it is sufficiently regular, it is strongly convex, and can be evaluated at any point of the domain. In addition to these, as has been mentioned above, the barycentric approximation gives in practice also a polynomial interpolation technique. For each of the four test functions f_k , we take N scattered points $\{x_i\}_{i=1}^N$, which are randomly selected from Ω , and construct the operator $BN[f_k]$. We then determine the mean square error (MSE) by evaluating

$$\frac{1}{N} \sum_{i=1}^N \frac{f_k(y_i) - BN[f_k](y_i)}{N}^2,$$

at N other randomly chosen points $y_i \in \Omega$ from Ω . The results are shown in Tables 3.1, 3.2, 3.3 and 3.4 clearly demonstrate that for all test functions f_k the MSE decreases with increasing numbers of nodes as N increases. It can also be observed from Figures 3.2 and 3.3, that the strong convexity of f_1 and f_2 has been preserved and there is almost no visual difference between the test function and its piecewise-linear interpolant. These examples are designed to follow the exact steps of methodology in this chapter.

Example 3.5.1 In the two following numerical tests for our barycentric approximation we will take the following two strongly convex functions.

$$f_1(x, y) \in 0.2(x - 0.4)^2 + (y - 0.5)^2 + 0.3 \exp((x - 0.5)^2 + (y - 0.5)^2),$$

and

$$f_2(x, y) \in 0.2(x - 0.4)^2 + (y - 0.5)^2,$$

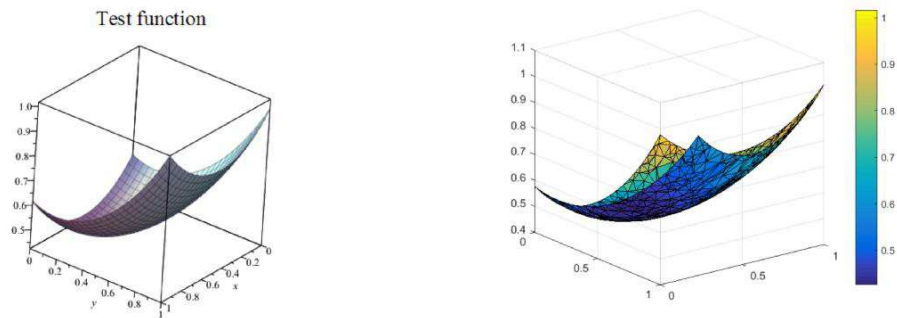
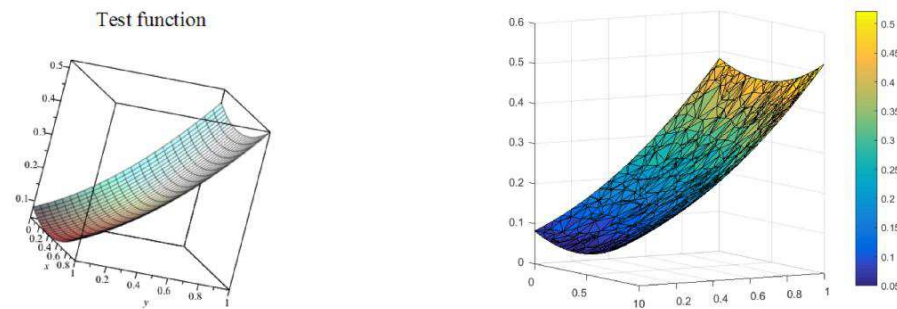
with the restriction of domain $D \in [0, 1] \times [0, 1]$. In both numerical tests, the data are generated from the above functions. However, the scattered points are chosen such that there exist 21 equally spaced nodes on each edge of the boundary of square D and 216 nodes in the square D . The nodes in the domain are positioned randomly chose from D while the nodes on the boundary is equally spaced. Figures 3.2 and 3.3 on the left are presented the graphs of f_1 and f_2 respectively, while Figures 3.2 and 3.3 on the right are described the graphs for linear interpolation of scattered data generated from the functions f_1 and f_2 respectively.

Table 3.1 – MSE for a function f_1 .

Function	Number of scatter data	N_w	MSE
$f_1(x, y)$	50	9	5.8×10^{i3}
	250	9	6.8005×10^{i4}
	1300	9	5.6326×10^{i5}

Table 3.2 – MSE for a function f_2 .

Function	Number of scatter data	N_w	MSE
$f_2(x, y)$	50	9	1.8×10^{i3}
	300	9	1.9338×10^{i4}
	700	9	6.4765×10^{i5}


Figure 3.2 – The figure on the left shows the graph of f_1 and the graph on the right for the piecewise-linear interpolation of the data generated from f_1 .

Figure 3.3 – The figure on the left shows the graph of f_2 and the graph on the right for the piecewise-linear interpolation of the data generated from f_2 .

On the approximation of strongly convex functions by an upper or lower operator

From Figs. 3.2 and 3.3 it is clear that the *strong* convexity of f_1 and f_2 has been preserved and there are no visual differences between the test functions and their linear interpolants.

Example 3.5.2 We take the following strongly convex function:

$$f_3(x, y, z) \in 0.1 \cdot (x - 0.4)^2 + (y - 0.5)^2 + (z - 0.3)^2,$$

the single-valued multivariate function above is defined in domain $(D \in [0,1] \times [0,1] \times [0,1])$, the accuracy of our approach illustrated here only by the tables (see the tables 3.3 and 3.4) of mean square error (MSE) for different numbers of scattered data for approximated functions. Note that the number of required scattered points increases in higher dimensions, in order to maintain the accuracy of the interpolated value.

Table 3.3 – MSE for a function f_3 .

Function	Number of scatter data	N_w	MSE
$f_3(x, y, z)$	200	1	1.193×10^{-1}
	400	1	8.26×10^{-2}
	8500	1	3×10^{-3}

Example 3.5.3 In the fourth example the data points is generated from the following test function:

$$f_4(x, y, z) \in 0.1 \cdot (x - 0.4)^2 + (y - 0.5)^2 + (z - 0.3)^2 + \exp(x - 0.5)^2$$

Table 3.4 – MSE for a function f_4 .

Function	Number of scatter data	N_w	MSE
$f_4(x, y, z)$	98	1	2.418×10^{-1}
	700	1	3.77×10^{-2}
	8500	1	3.5×10^{-3}



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4 Numerical integration under certain type of convexity

In this chapter, we shall extend some results of the papers [1, 2, 3, 4] by introducing a new class of cubature formulas for numerical integration (or multidimensional quadrature), that approximate from above (or from below) the exact value of the integrals of every function having a certain type of convexity. First, we would like to mention that all these papers were established in the context of the classical notion of convexity. Here, our objective is to extend the ideas given there under certain types of generalized convexity. To this end, this chapter is organized as follows: In Section 4.1, we first present some definitions, notations and then state two characterization results of any linear functional $C^{1,1}(-) \not\equiv \mathbf{R}$, which is nonnegative on the set of convex functions. We define two new classes of cubature formulas, which we call them strongly positive, respectively negative, definite cubature formulas. We then apply our general results to the case when the functional is the error functional of our cubature formulas. More precisely, we show that, for functions belonging to $C^{1,1}(-)$, the error estimates based on such cubature formulas may always controlled by the Lipschitz constants of the gradients, the different types of convexity and the error associated with using the quadratic function. In addition, knowing whether the function to be integrate satisfies the classical convexity or strong convexity, we establish sharp upper as well as lower refined bounds for the error estimates. In Section 4.2, for strongly positive definite cubature formulas, we establish characterization results between them and the partition of unity of the integration domain, but also show how we can construct them using decomposition method for domain integration. In Section 4.3, for strongly negative definite cubature formulas, we characterize them in two different ways: the first one by certain partitions of unity and the second one by a class of positive linear operators. Further, we show that there is a main difference between them and strongly positive definite cubature formulas. Indeed, we will show that the latter (strongly negative definite cubature formulas) can exist only if the domain of integration is a convex polytope. Finally, Section 4.4 will provide some numerical examples to illustrate the efficiency of our cubature formulas.

4.1 Notation, Terminology and preliminary results

We first introduce some notations, which follow closely those of [1, 2, 3]. Let Ω be a subset of $\mathbb{R}^d$. As usual, we mean by Ω° the interior of Ω . We say that Ω is *measurable* if it has a finite Lebesgue measure, which we denote by $|\Omega|$. For measurable Ω , the class $L^1(\Omega)$ comprises all Lebesgue integrable functions $f : \Omega \rightarrow \mathbb{R}$. A property holds *almost everywhere* (abbreviated by a.e.) on Ω if it holds on Ω except for a set of measure zero. Furthermore, we denote by $C(\Omega)$ the class of all real-valued continuous functions on Ω and by $C^k(\Omega)$, where $k \in \mathbb{N}$, the subclass of all functions which are k times continuously differentiable. It is convenient to agree that $C^0(\Omega) = C(\Omega)$. We continue to denote by $\|\cdot\|$ the Euclidean norm in $\mathbb{R}^d$ and $\langle \mathbf{x}, \mathbf{y} \rangle$ the standard inner product of $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.

We start by providing two characterization results of any linear functional $L : C^{1,1}(\Omega) \rightarrow \mathbb{R}$, which is nonnegative (or nonpositive) on the set of convex functions. We will be mainly interested in the case where the functional L is the remainder of our cubature formulas, as we will see later in this chapter. The first characterization is given in the following:

Lemma 4.1.1 *Let $\Omega \subset \mathbb{R}^d$ be a compact convex set. Let $L : C^k(\Omega) \rightarrow \mathbb{R}$, where $k \in \{0, 1\}$, be a linear functional, $\alpha \in \{1, -1\}$ and let ϵ be a positive real number. The two following statements are equivalent:*

(i) *For every convex function $f \in C(\Omega)$, we have*

$$\alpha L(f) \geq 0 \quad (4.1)$$

(ii) *For every ϵ -strongly convex function $g \in C(\Omega)$, we have*

$$\alpha L(g) \geq \frac{\epsilon}{2} \alpha L(\|\cdot\|^2) \quad (4.2)$$

Equalities are attained for all functions of the form

$$g(\mathbf{x}) = a(\mathbf{x}) + \frac{\epsilon}{2} \|\mathbf{x}\|^2,$$

where $a(\cdot)$ is any affine function.

Proof First we prove that (i) implies (ii). Let $g \in C(\Omega)$ be any ϵ -strongly convex function, since by Theorem 1.2.5, we know that

$$g + \frac{\epsilon}{2} \|\cdot\|^2$$

is convex function, then we can apply (4.1) to this function to immediately get

$$\alpha L\left(g + \frac{\epsilon}{2} \|\cdot\|^2\right) \geq 0.$$

Hence from linearity of R , we have

$$\frac{3}{4}R \left(g - \frac{1}{2} \right) \leq \frac{3}{4}R \left(k \cdot k^2 \right) \leq 0,$$

or equivalently

$$\frac{3}{4}R \left(g - \frac{1}{2} \right) \leq \frac{3}{4}R \left(k \cdot k^2 \right).$$

This shows that (ii) holds. Conversely, we now prove that (ii) implies (i). Let $f \in C^1(-)$ be any convex function, since

$$g : \mathbb{R} \rightarrow \mathbb{R} \text{ is } \frac{1}{2}\text{-strongly convex function, then we can apply (4.2) for this function to obtain}$$

$$\frac{3}{4}R \left(f - \frac{1}{2} \right) \leq \frac{3}{4}R \left(k \cdot k^2 \right),$$

thus, again using linearity of R , we have

$$\frac{3}{4}R \left(f - \frac{1}{2} \right) \leq \frac{3}{4}R \left(k \cdot k^2 \right) \leq \frac{3}{4}R \left(k \cdot k^2 \right).$$

Hence, the desired result of (ii) follows. ■

If in addition, the functions belong to $C^{1,1}(-)$, then our second characterization result is given in the following:

Lemma 4.1.2 Let $\mathbb{R}^d$ be a compact convex set. Let $R : C^k(-) \rightarrow \mathbb{R}$, where $k \in \{0, 1\}$, be a linear functional and let $\frac{3}{4} \in \{1, 1\}$. The two following statements are equivalent

(i) For every convex function $g \in C^{1,1}(-)$, we have

$$\frac{3}{4}R \left(g - \frac{1}{2} \right) \leq 0. \quad (4.3)$$

(ii) For every $f \in C^{1,1}(-)$ with $L(f)$ Lipschitz gradient, we have

$$\left| R \left(f - \frac{1}{2} \right) \right| \leq \frac{L(f)}{2}. \quad (4.4)$$

Equality is attained for all functions of the form

$$f(x) : \mathbb{R} \rightarrow \mathbb{R} \text{ is } a(x) + ck^2, \quad (4.5)$$

where $c \in \mathbb{R}$ and $a(x)$ is any affine function.

Proof First we prove (i) implies (ii). Let f be any function from $C^{1,1}(-)$ with Lipschitz constant

Numerical integration under certain type of convexity

$L(rf)$. Define the following two functions

$$g \in \mathcal{A}_{k,k^2}^{L(rf)} \text{ and } f \in \mathcal{A}_{k,k^2}^{L(rf)}.$$

Then, according to [4, proposition 2.2], we know that both of these functions belong to $C^{1,1}(-)$ and are also convex. Hence, by (4.3), we have

$$\mathbb{E} \left[\frac{1}{2} R(g) \right] \geq 0.$$

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

$$\mathbb{E} \left[\frac{1}{2} R(g) \right] = \frac{1}{2} R(g) \cdot \mathbb{E} \left[\frac{1}{2} R(f) \right] + \mathbb{E} \left[\frac{1}{2} R(g) \right] \cdot \frac{1}{2} R(f).$$

This is equivalent to (4.4).

For the statement on the occurrence of equality, it is enough to note that a linear functional R satisfying (4.3) for all convex functions must vanish for affine functions. Now, let us assume that (ii) holds. Then, we deduce that

$$\mathbb{E} \left[\frac{1}{2} R(g) \right] = 0, \quad \text{and that} \quad (4.6)$$

$$\mathbb{E} \left[\frac{1}{2} R(f) \right] = 0. \quad (4.7)$$

Let $g \in C^{1,1}(-)$ be any convex function and set

$$f \in \mathcal{A}_{k,k^2}^{L(rg)} \text{ and } g \in \mathcal{A}_{k,k^2}^{L(rg)}.$$

Then, according to [4, proposition 2.2], we have

$$f \in C^{1,1}(-) \text{ and } L(rf) = L(rg). \quad (4.8)$$

Since

$$g \in \mathcal{A}_{k,k^2}^{L(rg)} \text{ and } f \in \mathcal{A}_{k,k^2}^{L(rg)},$$

it can be written as follows

$$g \in \mathcal{A}_{k,k^2}^{L(rf)} \text{ and } f \in \mathcal{A}_{k,k^2}^{L(rf)}.$$

we therefore obtain

$$\frac{3}{4}R(g) \leq \frac{3}{4}R(k,k^2) \frac{L(f)}{L(g)} \leq \frac{3}{4}R(k,k^2) \frac{L(f)}{L(g)}.$$

Finally, by combining (4.6), (4.7) and (4.8) we can conclude that (i) is valid. ■

We now define our new general class of cubature formulas, which we formulate as follows:

Definition 4.1.3 Let $\Omega \subset \mathbb{R}^d$ be a compact set and let α be a positive real number. For n points $x_1, \dots, x_n \in \Omega$, called nodes, and associated positive numbers $A_1, \dots, A_n$, we say that

$$(A_i, x_i) : i \in \{1, \dots, n\}, \quad (4.9)$$

defines the α -strongly definite cubature formula

$$\int_{\Omega} f(x) dx \leq \sum_{i \in \{1, \dots, n\}} A_i f(x_i) \leq \frac{1}{\alpha} \int_{\Omega} f(x) dx, \quad (4.10)$$

if there exists $\beta \in \{1, 1\}$ such that

$$\frac{1}{\alpha} \int_{\Omega} f(x) dx \leq \frac{1}{\beta} \int_{\Omega} f(x) dx, \quad (4.11)$$

for all α -strongly convex functions $f \in C(\Omega)$.

In the case of $\alpha \in \{1, 1\}$, we say that (4.10) is a α -strongly positive definite cubature formula or a α -strongly pd-formula for short. We also call (4.9) a α -strongly pd-system, which is said to be of length n if the points $x_1, \dots, x_n$ are distinct.

For $\alpha \in \{1, 1\}$, a corresponding terminology is used with 'positive' replaced by 'negative' and 'pd' replaced by 'nd'.

Remark 4.1.4 Note that a α -strongly positive or negative definite cubature formula as specified in Definition 4.1.3 is always of order two. In fact, by Lemma 4.1.2 inequality (4.4) the functional R vanishes for affine functions and so the order is at least two. However, if the order were greater than two, then (4.4) would imply that $R(f) \leq 0$ for all $f \in C^{1,1}(\Omega)$. Recall that, in the univariate case, a quadrature rule is strongly positive definite or strongly negative definite if and only if its second Peano kernel is greater than zero or less than zero, respectively; see [5, Chap. I 4] or [6, Chap. 4.3].

In the theory of inequalities, inequality (4.11), with R defined by (4.10) and valid for all α -strongly convex functions, has also been called lower (resp., an upper) **Hermite-Hadamard inequality** when $\alpha \in \{1, 1\}$ (resp., $\alpha \in \{1, 1\}$). It is clear, because every strongly convex function is convex function, by using [7, Theorem 2.3] that the upper Hermite-Hadamard inequalities or, equivalently, α -strongly negative definite cubature formulas, can exist only when Ω is a compact convex polytope.

We now present a characterization of our class of cubature formulas in terms of their associated error functionals. Indeed, we show that for functions in $C^{1,1}(\cdot)$, the error estimates based on such cubature formulas are always controlled by the Lipschitz constants of the gradients, the strong convexity parameter and the error associated with using the quadratic function. This result is a direct consequence of Lemmas 4.1.1 and 4.1.2.

Theorem 4.1.5 *Let $\Omega \subset \mathbb{R}^d$ be a compact convex set. A cubature formula (4.10) is 1 -strongly positive or negative definite if and only if for all $f \in C^{1,1}(\cdot)$, the error functional associated to the cubature formula satisfies*

$$\frac{1}{2} \sum_{k=1}^n \lambda_k \left(\int_{\Omega} f(x) dx - \sum_{i=1}^m \alpha_i f(x_i) \right)^2 \leq \frac{L^2}{2} \sum_{k=1}^n \lambda_k \|x_k - \bar{x}\|^2, \quad (4.12)$$

with $\lambda_k \in [0, 1]$ or $\lambda_k \in [-1, 0]$, respectively. In (4.12), equality is attained for all functions of the form

$$f(x) = a(x) + \frac{1}{2} \|x - x_0\|^2,$$

where $a(\cdot)$ is any affine function.

4.2 Strongly positive definite cubature formulas

4.2.1 Construction and Characterization of Strongly Positive Definite Cubature Formulas

Our first construction method of strongly positive definite cubature formulas is based on domain decomposition of the domain of integration, which we define as follows:

Definition 4.2.1 *Let $\Omega \subset \mathbb{R}^d$ be a measurable set of finite positive measure. A system $\{\Omega_1, \dots, \Omega_n\}$ of subsets is called a **decomposition** of Ω if :*

- (i) Ω_i is measurable and $|\Omega_i| \geq 0$ for $i \in \{1, \dots, n\}$;
- (ii) $|\Omega_i \cap \Omega_j| = 0$ if $i \neq j$;
- (iii) $\Omega = \bigcup_{i=1}^n \Omega_i$.

Our first construction method is given by the following Theorem.

Theorem 4.2.2 *Let $\Omega \subset \mathbb{R}^d$ be a compact convex set of positive measure and let $\{\Omega_1, \dots, \Omega_n\}$ be a decomposition of Ω . Set*

$$A_i = |\Omega_i| \text{ and } x_i \in \Omega_i \text{ and } \lambda_i = \frac{1}{|\Omega|} |\Omega_i| \quad (i \in \{1, \dots, n\}).$$

Then, for any $\epsilon \in (0, 1)$, $\{(A_i, \mathbf{x}_i) : i \in 1, \dots, n\}$ defines a ϵ -strongly positive definite cubature formula on $\mathbb{R}^d$.

Proof Since $\mathbb{R}^d$ is convex, it is easy to see that $\mathbf{x}_i \in \mathbb{R}^d$; however, $\mathbf{x}_i$ need not lie in $\mathbb{R}^d$. Now, let $f \in C(\mathbb{R}^d)$ be ϵ -strongly convex function. Then at each point $y \in \mathbb{R}^d$, the graph of f is supported from below by hyperplane [8, Definition 2.1.2, p.63]. In particular, there exist vectors $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n \in \mathbb{R}^d$ such that

$$f(\mathbf{x}) \geq f(\mathbf{x}_i) + \langle \mathbf{a}_i, \mathbf{x} - \mathbf{x}_i \rangle + \frac{\epsilon}{2} \|\mathbf{x} - \mathbf{x}_i\|^2, \quad (i \in 1, \dots, n). \quad (4.13)$$

Integrating both sides over $\mathbb{R}^d$ and noting that

$$\int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x} \geq \int_{\mathbb{R}^d} f(\mathbf{x}_i) d\mathbf{x} + \langle \mathbf{a}_i, \int_{\mathbb{R}^d} (\mathbf{x} - \mathbf{x}_i) d\mathbf{x} \rangle + \frac{\epsilon}{2} \int_{\mathbb{R}^d} \|\mathbf{x} - \mathbf{x}_i\|^2 d\mathbf{x},$$

and because, we have

$$\int_{\mathbb{R}^d} (\mathbf{x} - \mathbf{x}_i) d\mathbf{x} = 0,$$

then, we conclude that

$$\int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x} \geq f(\mathbf{x}_i) \int_{\mathbb{R}^d} d\mathbf{x} + \frac{\epsilon}{2} \int_{\mathbb{R}^d} \|\mathbf{x} - \mathbf{x}_i\|^2 d\mathbf{x}. \quad (4.14)$$

In view of the fact that

$$\|\mathbf{x} - \mathbf{x}_i\|^2 \leq \|\mathbf{x}\|^2 + 2\langle \mathbf{x}, \mathbf{x}_i \rangle + \|\mathbf{x}_i\|^2,$$

it follows that

$$\begin{aligned} \int_{\mathbb{R}^d} \|\mathbf{x} - \mathbf{x}_i\|^2 d\mathbf{x} &\leq \int_{\mathbb{R}^d} \|\mathbf{x}\|^2 d\mathbf{x} + 2 \int_{\mathbb{R}^d} \langle \mathbf{x}, \mathbf{x}_i \rangle d\mathbf{x} + \int_{\mathbb{R}^d} \|\mathbf{x}_i\|^2 d\mathbf{x} \\ &\leq \int_{\mathbb{R}^d} \|\mathbf{x}\|^2 d\mathbf{x} + 2 \int_{\mathbb{R}^d} \langle \mathbf{x}, \mathbf{x}_i \rangle d\mathbf{x} + \int_{\mathbb{R}^d} \|\mathbf{x}_i\|^2 d\mathbf{x} \\ &\leq \int_{\mathbb{R}^d} \|\mathbf{x}\|^2 d\mathbf{x} + 2 \int_{\mathbb{R}^d} \langle \mathbf{x}, \mathbf{x}_i \rangle d\mathbf{x} + \int_{\mathbb{R}^d} \|\mathbf{x}_i\|^2 d\mathbf{x} \\ &\leq \int_{\mathbb{R}^d} \|\mathbf{x}\|^2 d\mathbf{x} + 2 \int_{\mathbb{R}^d} \langle \mathbf{x}, \mathbf{x}_i \rangle d\mathbf{x} + \int_{\mathbb{R}^d} \|\mathbf{x}_i\|^2 d\mathbf{x} \\ &\leq \int_{\mathbb{R}^d} \|\mathbf{x}\|^2 d\mathbf{x} + 2 \int_{\mathbb{R}^d} \langle \mathbf{x}, \mathbf{x}_i \rangle d\mathbf{x} + \int_{\mathbb{R}^d} \|\mathbf{x}_i\|^2 d\mathbf{x}. \end{aligned} \quad (4.15)$$

Thus from (4.14), we have

$$\int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x} \geq f(\mathbf{x}_i) \int_{\mathbb{R}^d} d\mathbf{x} + \frac{\epsilon}{2} \left(\int_{\mathbb{R}^d} \|\mathbf{x}\|^2 d\mathbf{x} - \int_{\mathbb{R}^d} \|\mathbf{x}_i\|^2 d\mathbf{x} \right).$$

Hence, summing over i from 1 to n , we arrive at

$$\sum_{i \in I} \frac{1}{n} \left(\int_{\Omega} \frac{1}{k_i k_j^2} d\mathbf{x} \right) \mathbf{x}_i^n \sum_{j \in I} A_j k_j k_i^2,$$

or, equivalently,

$$\sum_{i \in I} \frac{1}{n} \left(\int_{\Omega} \frac{1}{k_i k_j^2} d\mathbf{x} \right) \mathbf{x}_i^n \sum_{j \in I} A_j k_j k_i^2.$$

Finally, we may conclude as required that

$$R^{\frac{1}{2}} f^{\frac{1}{2}} \leq \frac{1}{2} R^{\frac{1}{2}} k_i k_j^2.$$

■

In order to describe the second constructive method, we introduce the following notion.

Definition 4.2.3 Let $\Omega \subset \mathbb{R}^d$ be a measurable set of finite positive measure. A system $\{f_1, \dots, f_n\}$ of real-valued functions is called a **partition of unity** on Ω if:

- (i) $f_i \in L^1(\Omega)$ and $\int_{\Omega} f_i(\mathbf{x}) d\mathbf{x} \geq 0$ for $i \in \{1, \dots, n\}$;
- (ii) $f_i(\mathbf{x}) \geq 0$ a.e. on Ω , for $i \in \{1, \dots, n\}$;
- (iii) $f_1(\mathbf{x}) + \dots + f_n(\mathbf{x}) = 1$ a.e. on Ω .

Our second construction method is given by the following Theorem.

Theorem 4.2.4 Let $\Omega \subset \mathbb{R}^d$ be a compact convex set of positive measure and let $\{f_1, \dots, f_n\}$ be a partition of unity on Ω . Set

$$A_i := \int_{\Omega} f_i(\mathbf{x}) d\mathbf{x} \quad \text{and} \quad \mathbf{x}_i := \frac{1}{A_i} \int_{\Omega} \mathbf{x} f_i(\mathbf{x}) d\mathbf{x} \quad (i \in \{1, \dots, n\}).$$

Then $\{(A_i, \mathbf{x}_i) : i \in \{1, \dots, n\}\}$ defines a 1 -strongly positive definite cubature formula on Ω .

Proof The proof is very similar to that of Theorem 4.2.2. Again, we first observe that $x_i \geq 0$ for $i \in \{1, \dots, n\}$. Hence, for any 1 -strongly convex function $f \in C(\Omega)$, there hold n inequalities of the form (4.13). They are preserved if we multiply both sides by f_i and integrate over Ω . Actually, in the present case we immediately get

$$\int_{\Omega} f(\mathbf{x}) f_i(\mathbf{x}) d\mathbf{x} \geq f(\mathbf{x}_i) \int_{\Omega} f_i(\mathbf{x}) d\mathbf{x} \geq A_i f(\mathbf{x}_i) \geq \frac{1}{2} \int_{\Omega} f_i(\mathbf{x}) k_{\mathbf{x}_i} k_{\mathbf{x}_j}^2 d\mathbf{x}.$$

In view of

$$\int_{\Omega} (x_i - x_j)^2 f(x) dx \geq 0,$$

then,

$$\int_{\Omega} f(x) f(x_j) dx - f(x_j) \int_{\Omega} f(x) dx \leq \frac{1}{2} \int_{\Omega} (x_i - x_j)^2 f(x) dx,$$

or equivalently

$$\int_{\Omega} f(x) f(x) dx - A_j f(x_j) \leq \frac{1}{2} \int_{\Omega} (x_i - x_j)^2 f(x) dx. \quad (4.16)$$

Since, we know that

$$k_{x_i, x_j}^2 \leq k_{x_i, x_i}^2 \leq 2h_{x_i, x_j} \leq k_{x_j, x_j}^2,$$

then

$$\int_{\Omega} k_{x_i, x_j}^2 f(x) dx \leq \int_{\Omega} k_{x_i, x_i}^2 f(x) dx \leq 2 \int_{\Omega} h_{x_i, x_j} f(x) dx \leq \int_{\Omega} k_{x_j, x_j}^2 f(x) dx \quad (4.17)$$

$$\leq \int_{\Omega} k_{x_i, x_j}^2 f(x) dx \leq 2 \int_{\Omega} h_{x_i, x_j} f(x) dx \leq \int_{\Omega} k_{x_j, x_j}^2 f(x) dx$$

$$\leq \int_{\Omega} k_{x_i, x_j}^2 f(x) dx \leq 2h_{x_i, x_j} A_j \leq \int_{\Omega} k_{x_j, x_j}^2 f(x) dx$$

$$\leq \int_{\Omega} k_{x_i, x_j}^2 f(x) dx \leq 2A_j k_{x_i, x_j}^2 \leq \int_{\Omega} k_{x_j, x_j}^2 f(x) dx$$

$$\leq \int_{\Omega} k_{x_i, x_j}^2 f(x) dx \leq A_j k_{x_j, x_j}^2.$$

Then (4.17) may simply rewritten as follows

$$\int_{\Omega} k_{x_i, x_j}^2 f(x) dx \leq \int_{\Omega} k_{x_i, x_i}^2 f(x) dx \leq A_j k_{x_j, x_j}^2.$$

Hence, from (4.16), we conclude

$$\int_{\Omega} f(x) f(x_j) dx - A_j f(x_j) \leq \frac{1}{2} \left(\int_{\Omega} k_{x_i, x_j}^2 f(x) dx + A_j k_{x_j, x_j}^2 \right).$$

Finally, summing over i from 1 to n , we arrive at

$$\int_{\Omega} f(x) f(x) dx - \frac{1}{n} \left(\int_{\Omega} f(x) dx \right)^2 \leq \frac{1}{2n} \left(\int_{\Omega} k_{x_i, x_j}^2 f(x) dx + A_j k_{x_j, x_j}^2 \right).$$

We conclude that

$$\int_{\Omega} f(x) f(x) dx - \frac{1}{n} \left(\int_{\Omega} f(x) dx \right)^2 \leq \frac{1}{2n} \left(\int_{\Omega} k_{x_i, x_j}^2 f(x) dx + A_j k_{x_j, x_j}^2 \right).$$

Or equivalently as required

$$R^1 f^2 \leq \frac{1}{2} R^1 k \cdot k^2.$$

■

Remark 4.2.5 The function $'_i$ of a partition of unity can be interpreted physically as a distribution of mass on $-$. Then A_i of Theorem 4.2.4 is the total mass and $\mathbf{x}_i$ is the center of mass or center of gravity with respect to $'_i$.

Remark 4.2.6 Note that every 1 -strongly positive definite cubature formula which is generated by a decomposition of the domain $-$ can also be obtained by a partition of unity. In fact, let $\{-_1, \dots, -_n\}$ be a decomposition of $-$. For $i \in 1, \dots, n$, define

$$'_i(\mathbf{x}) := \frac{m(\mathbf{x})}{m_i} \quad \text{if } \mathbf{x} \in -_i, \quad (4.18)$$

$$m(\mathbf{x}) := \sum_{j=1}^n m_j$$

where $m(\mathbf{x})$ is the number of subsets $-_1, \dots, -_n$ that contain $\mathbf{x}$. Then

$$\sum_{i=1}^n '_i(\mathbf{x}) \in 1 \quad \text{for } \mathbf{x} \in -, \quad (4.19)$$

and so $\{'_1, \dots, '_n\}$ is a partition of unity that generates the same 1 -strongly positive definite cubature formula as $\{-_1, \dots, -_n\}$. Moreover, instead of (4.18), we can define $'_i$ to be the characteristic function of $-_i$ with respect to $-$ since it suffices that (4.19) holds almost everywhere on $-$. In view of the last observation, it seems to be reasonable to identify two partitions of unity that differ on sets of measure zero only.

Remark 4.2.6 shows that by partitions of unity we can construct at least as many 1 -strongly positive definite cubature formulas as by decompositions of $-$. We may therefore ask whether there are still 1 -strongly positive definite cubature formulae that cannot be generated by a partition of unity. The answer is **no**. In fact, the following converse of Theorem 4.2.4 is true. Of course, it also gives another justification of Remark 4.2.6. The proof of this result is essentially based on [2, Theorem 3.8, p.269].

Theorem 4.2.7 Let $-\frac{1}{2} \mathbf{R}^d$ be a compact convex set of positive measure. Suppose that $\{(A_i, \mathbf{x}_i) : i \in 1, \dots, n\}$ defines a 1 -strongly positive definite cubature formula on $-$. Then there exists a partition of unity $\{'_1, \dots, '_n\}$ on $-$ such that

$$\sum_{i \in 1}^n A_i \int - '_i(\mathbf{x}) d\mathbf{x} \quad \text{and} \quad \sum_{i \in 1}^n \frac{1}{A_i} \int - \mathbf{x}_i '_i(\mathbf{x}) d\mathbf{x} \quad (i \in 1, \dots, n).$$

Proof Let us assume that

$$\{(A_i, \mathbf{x}_i) : i \in 1, \dots, n\}$$

4.3. Strongly Negative Definite Cubature Formulas

defines a τ -strongly positive definite cubature formula on Ω . Then by definition, for any τ -strongly convex function f , we have

$$R_{\tau} f \geq \frac{1}{2R} \sum_{k=1}^n k^2 f(x_k), \quad (4.20)$$

where

$$f(x) d\mathbf{x} \in \mathbb{R}^d, \quad \sum_{i=1}^n A_i f(x_i) \approx R f.$$

According to Lemma 4.1.1, we have, for every convex function $g \in C(\Omega)$,

$$R g \geq 0. \quad (4.21)$$

This means that, for every convex function $g \in C(\Omega)$,

$$\sum_{i=1}^n g(x_i) \geq \sum_{i=1}^n A_i g(x_i).$$

Hence, by [2, Theorem 3.8, p.269], there exists a partition of unity $\{1, \dots, n\}$ on Ω such that

$$A_i \in \mathbb{R}^d, \quad \sum_{i=1}^n A_i = \mathbf{1} \quad \text{and} \quad x_i \in \Omega, \quad \sum_{i=1}^n A_i x_i = \mathbf{0} \quad (i \in 1, \dots, n).$$

This shows the required property and completes the proof. ■

4.3 Strongly Negative Definite Cubature Formulas

In this section, we will emphasize on some valuable results about strongly negative definite cubature formulas (see Definition 4.1.3). We also show the main difference between them and strongly positive definite cubature formulas. As we will see, compared to the latter, here the domain of integration $\Omega \subset \mathbb{R}^d$ must be a compact convex polytope with positive measure. In particular, we characterize such a class of cubature formulas by certain partitions of unity or, alternatively, by a class of positive linear operators.

However, one might suspect that the results on τ -strongly pd-formulas can be easily transferred to results on τ -strongly nd-formulas but, apart from the fact that their respective error terms can be controlled from above and below (see Theorem 4.1.5), there is not much analogy between the two types of cubature formulas. As we will see below, already the question of *existence* shows significant differences while τ -strongly pd-formulas exist for all compact convex sets Ω , the existence of an τ -strongly nd-formula requires Ω to be a convex polytope whose vertices are among the nodes. This result can be derived from (4.22) of Theorem 4.3.1

4.3.1 Characterization of Strongly Negative Definite Cubature Formulas

From now on let $\omega \subset \mathbb{R}^d$ be a compact convex polytope of positive measure, and let $X \subseteq \omega$ be a finite subset that includes the vertices of ω . Thus, the convex hull of X must be equal to ω . Now, we can characterize strongly negative definite cubature formulas by using some arguments essentially based on the paper [3, Theorem 2.1a, p.97 and Theorem 2.1b, p.99].

Theorem 4.3.1 *A set $\alpha \subseteq \{(A_i, x_i) : i \in 1, \dots, n\}$ defines a 1 -strongly negative definite cubature formula on ω if and only if there exists a **partition of unity** $\{\hat{A}_1, \dots, \hat{A}_n\}$ on ω such that*

$$\sum_{i \in 1}^n \hat{A}_i(x) x_i \quad (\text{a.e. on } \omega), \quad (4.22)$$

and

$$\int_{\omega} \hat{A}_i(x) dx = A_i \quad (i \in 1, \dots, n). \quad (4.23)$$

Proof Let $\alpha \subseteq \{(A_i, x_i) : i \in 1, \dots, n\}$ defines a 1 -strongly negative definite cubature formula on ω . Then, according to the definition the error functional R satisfies, for any 1 -strongly convex function f , we have

$$R(f) \leq - \frac{1}{2} R(k^2). \quad (4.24)$$

We deduce then from Lemma 4.1.1 that, for every convex function $g \in C(\omega)$, we have

$$R(g) \geq 0. \quad (4.25)$$

This means that the estimate

$$\int_{\omega} g(x) dx \leq \sum_{i \in 1}^n A_i g(x_i),$$

holds for every convex function $g \in C(\omega)$. Hence by [3, Theorem 2.1a, p.97], there exists a partition of unity $\{\hat{A}_1, \dots, \hat{A}_n\}$ on ω , which satisfies the required conditions (4.22) and (4.23).

Conversely, assume that there exists a partition of unity $\{\hat{A}_1, \dots, \hat{A}_n\}$ on ω , such that conditions (4.22) and (4.23) hold. Let f be convex on ω . Then, from (4.22) and convexity of f we deduce that

$$f(x) \leq \sum_{i \in 1}^n \hat{A}_i(x) f(x_i).$$

Integrating both sides over ω and using (4.23), we obtain the inequality

$$\int_{\omega} f(x) dx \leq \sum_{i \in 1}^n A_i f(x_i).$$

Since the above inequality holds for every convex function, then according to Lemma 4.1.1 we

4.3. Strongly Negative Definite Cubature Formulas

also have, for every λ -strongly convex function,

$$\int_{\mathbb{R}^n} f(x) d\mu(x) \geq \frac{1}{2} \int_{\mathbb{R}^n} k(x) d\mu(x). \quad (4.26)$$

This shows that $\{(A_i, x_i) : i \in 1, \dots, n\}$ defines a λ -strongly negative definite cubature formula on $\mathbb{R}^n$.

Remark 4.3.2 Comparing Theorem 4.3.1 with Theorem 4.2.7, we see an essential difference between λ -strongly nd- and pd-formulas. Indeed, while **every** partition of unity produces a λ -strongly pd-formula, we need the additional condition (4.22) for producing an λ -strongly nd-formula. Moreover, if (4.22) and (4.23) hold, and we introduce

$$y_i \in \overline{A} \quad \int_{\mathbb{R}^n} x A_i(x) d\mu(x) \in \frac{\int_{\mathbb{R}^n} x A_i(x) d\mu(x)}{\int_{\mathbb{R}^n} A_i(x) d\mu(x)} \quad (i \in 1, \dots, n),$$

then $y_i \in \mathbb{R}^n$, since it has been represented as convex combination of points of $\mathbb{R}^n$. Then, it can be easily verified that, for all λ -strongly convex functions $f \in C(\mathbb{R}^n)$, the following estimates hold:

$$\int_{\mathbb{R}^n} A_i f(y_i) d\mu(x) \leq \int_{\mathbb{R}^n} f(x) d\mu(x) + \int_{\mathbb{R}^n} A_i^T(x) d\mu(x).$$

Hence, every λ -strongly nd-formula generates a λ -strongly pd-formula.

Recall that a linear operator L that maps $C(\mathbb{R}^n)$ into a linear space of functions $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is called **positive** if $f \geq 0$ implies $L f \geq 0$ almost everywhere on $\mathbb{R}^n$. Furthermore, L is said to be of **linear precision** if for each affine function a , we have $L[a](x) = a(x)$ almost everywhere on $\mathbb{R}^n$.

The following result provides another characterization of a λ -strongly negative definite cubature formula in terms of the existence of a certain positive linear operator, which satisfies the linear precision property.

Theorem 4.3.3 A set $a \in \{(A_i, x_i) : i \in 1, \dots, n\}$ defines a λ -strongly negative definite cubature formula on $\mathbb{R}^n$ if and only if there exists a **positive linear operator** L of linear precision, of the form

$$L f(x) = \sum_{i=1}^n A_i(x) f(x_i),$$

with $A_i \in L^1(\mathbb{R}^n)$ and $A_i \in \mathbb{R}^n$ - $\int_{\mathbb{R}^n} A_i(x) d\mu(x) \in 0$ for $i \in 1, \dots, n$.

Proof The proof is very similar to the proof of Theorem 4.3.1. Then $\{(A_i, x_i) : i \in 1, \dots, n\}$ defines a negative definite cubature formula on $\mathbb{R}^n$. Hence by [3, Theorem 2.1b, p.99], there

exists a positive linear operator L of linear precision, of the form

$$L f(x) = \sum_{i=1}^n A_i(x) f(x_i),$$

with $A_i \in L^1(\cdot)$ and $A_i(x) \geq 0$ for $i = 1, \dots, n$.

Conversely, assume that there exists a positive linear operator L of linear precision, of the form that above. Let f be convex on Δ . Then, from the form of $L f(x)$ and convexity of f we deduce

$$f(x) \leq \sum_{i=1}^n A_i(x) f(x_i).$$

Integrating both sides over Δ , we obtain the inequality

$$\int_{\Delta} f(x) dx \leq \sum_{i=1}^n \left(\int_{\Delta} A_i(x) dx \right) f(x_i).$$

Since the above inequality holds for every convex function, then according to Lemma 4.1.1 we also have, for every λ -strongly convex function,

$$\int_{\Delta} f(x) dx \leq \frac{1}{2} \sum_{i=1}^n \left(\int_{\Delta} A_i(x) dx \right) k^2.$$

This shows that $\{(A_i, x_i) : i = 1, \dots, n\}$ defines a λ -strongly negative definite cubature formula on Δ .

4.3.2 Practical Construction of Strongly Negative Definite Cubature Formulas

We now turn to a practical construction of strongly negative definite cubature formulas. To this end, let us first consider the case where Δ is a non-degenerate simplex in $\mathbb{R}^d$ with vertices $x_i, i = 1, \dots, d+1$, being the set of its vertices. Then each $x \in \Delta$ has a unique representation as a convex combination

$$x = \sum_{i=1}^{d+1} \lambda_i(x) x_i,$$

where λ_i is the restriction to Δ of the affine function that attains the value 1 at x_i and is zero at all the other vertices of Δ . The value $\lambda_i(x)$ is the **barycentric co-ordinate** of x with respect to x_i . According to [7, Theorem 2.2]), we know that for every convex function f on Δ , it holds

$$\int_{\Delta} f(x) dx \leq \frac{1}{d+1} \sum_{i=1}^{d+1} f(x_i).$$

X

Consequently, by Lemma 4.1.1, the system $\lambda_1, \dots, \lambda_{d+1}$ produces the strongly λ -system

$$\left\{ \frac{1}{d+1} \lambda_i, x_i : i = 1, \dots, d+1 \right\}.$$

It is the only strongly nd-system on Ω which has no other nodes than the vertices.

Now let $\mathbf{X} \in \bigotimes_{i=1}^n \mathbf{R}^d, i \in 1, \dots, n$ be an arbitrary set of points of $\mathbf{R}^d$. The previous approach can be generalized when $\Omega \in \text{conv}(\mathbf{X})$ is an arbitrary polytope in $\mathbf{R}^d$. A **triangulation** T of Ω with respect to $\mathbf{X}$ is a decomposition of Ω into d -dimensional simplices such that $\mathbf{X}$ is the set of all their vertices, and the intersection of any two simplices consists of a common lower-dimensional simplex or is empty. Triangulations of compact convex polytopes exist.¹

Indeed, given any finite set $\mathbf{X}$ of points that do not all lie on a hyperplane, Chen and Xu [9, p. 301] describe a lifting-and-projection procedure which results in a triangulation of the convex hull of $\mathbf{X}$ with respect to $\mathbf{X}$. For an explicit statement on the existence of triangulations with a proof based on an algorithmic method, see [10, Theorem 3, part a].

Now let $\mathbf{S}_1, \dots, \mathbf{S}_l$ be the simplices of T , and let N_i be the set of all integers j such that $\mathbf{x}_j$ is a vertex of $\mathbf{S}_i$. If $\mathbf{x} \in \mathbf{S}_j$ and $j \in N_i$, then we denote by $s_{ij}(\mathbf{x})$ the barycentric co-ordinate of $\mathbf{x}$ with respect to $\mathbf{x}_i$ for the simplex $\mathbf{S}_j$. It is easily verified that if $\mathbf{x} \in \mathbf{S}_j \cap \mathbf{S}_k$, then $s_{ij}(\mathbf{x}) \in s_{ik}(\mathbf{x})$ if $j, k \in N_i$ and $s_{ij}(\mathbf{x}) \in 0$ if $j \in N_i, k \notin N_i$. Therefore, setting

$$A_i(\mathbf{x}) := \begin{cases} s_{ij}(\mathbf{x}) & \text{if } \mathbf{x} \in \mathbf{S}_j \text{ and } j \in N_i \\ 0 & \text{otherwise} \end{cases}$$

:

for $i \in 1, \dots, n$, we obtain a well-defined partition of unity $A_1, \dots, A_n$ that satisfies (4.22). This obviously produces the strongly nd-formula

$$\int_{\Omega} f(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \sum_{i=1}^n A_i(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} = \sum_{i=1}^n \int_{\Omega} A_i(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} \quad (4.27)$$

4.4 Numerical Examples

In order to give numerical illustrations of the effectiveness of our application of the strongly nd-formula (4.27) with triangulations created using Delaunay Triangulation. We apply it to approximate the integrals of three real-valued (test) functions of multiple variables $f_k, k \in 1, 2, 3$, when the domain Ω is a square, and f_k possess the following features: it is sufficiently regular, it is strongly convex or convex, and can be evaluated at any point of the domain. For each of the three test functions f_k , we take N scattered points $\{\mathbf{x}_i\}_{i=1}^N$, which are randomly selected from Ω and construct the cubature formula $\int_{\Omega} f(\mathbf{x}) d\mathbf{x} \approx \sum_{i=1}^N A_i f(\mathbf{x}_i)$ given as in (4.27). We then determine

$$\text{the error } R_f \text{ by evaluating } R_f = \left| \int_{\Omega} f(\mathbf{x}) d\mathbf{x} - \sum_{i=1}^N A_i f(\mathbf{x}_i) \right|$$

The results are shown in Tables 4.1, 4.2 and 4.3 clearly demonstrate that for all test functions f_k the error R_f decreases with increasing numbers of nodes as N increases. It can also be

¹ It seems that in dimension $d \in 3$ the existence was already known to mathematicians like Euler and Dirichlet.

Numerical integration under certain type of convexity

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observed from Figures 4.7, 4.8 and 4.9 the “best fit” lines for the error $R f_k$ which were found by using least squares regression or linear regression. These examples are designed to follow the exact steps of methodology in this chapter.

Example 4.4.1 In the two following numerical tests for our cubature formula (numerical integration) we will take the following two strongly convex functions.

$$f_1(x, y) \in 0.2 \cdot (x - 0.4)^2 \cdot (y - 0.5)^2 \cdot \exp((x - 0.5)^2 \cdot (y - 0.5)^2),$$

and

$$f_2(x, y) \in 0.2 \cdot (x - 0.4)^2 \cdot (y - 0.5)^2,$$

with the restriction of domain $D : \in [0, 1] \times [0, 1]$. In both numerical tests, the data are generated from the above functions. However, the scattered points are chosen such that there exist 2 equally spaced nodes on each edge of the boundary of square D and N nodes in the square D . The nodes in the domain are positioned randomly chose from D while the nodes on the boundary is equally spaced. Figures 4.1 and 4.3 are presented the error of numerical integration of f_1 and f_2 respectively. While Figures 4.2 and 4.4 are presented the error of numerical integration of f_1 and f_2 in terms of the log scale respectively.

The exact value of the integration to the function $f_1(x, y)$ is equal to 0.591746465805074

Table 4.1 – The error of numerical integration for function f_1 .

Function	Number of scattered points	Numerical integration values	Error
f_1	54	0.606048591515064	$1.43021257099898 \times 10^{-2}$
	504	0.593436541476951	$1.69007567187685 \times 10^{-3}$
	1004	0.592681353963911	$9.34888158837022 \times 10^{-4}$
	10004	0.591841309865544	$9.48440604706668 \times 10^{-5}$

Now, we take the second strongly convex function:

$$f_2(x, y) \in 0.2 \cdot (x - 0.4)^2 \cdot (y - 0.5)^2.$$

The exact value of the integration to the function $f_2(x, y)$ is equal to 0.235333333333333

4.4. Numerical Examples

Table 4.2 – The error of numerical integration for function f_2 .

Function	Number of scattered points	Numerical integration values	Error
f_2	54	0.239885403766284	$4.55207043295111 \times 10^{-3}$
	504	0.235867353761321	$5.34020427987864 \times 10^{-4}$
	3004	0.235430304103746	$9.69707704125411 \times 10^{-5}$

Example 4.4.2 In the following numerical test for our cubature formula (numerical integration) we will take the following convex function.

$$f_3(x, y) = x^3 + 5(y^2 - 0.6)^2 + 1.$$

with the restriction of domain $D : [0, 1] \times [0, 1]$. In the following numerical test, the data are generated from the above function. However, the scattered points are chosen such that there exist 2 equally spaced nodes on each edge of the boundary of square D and N nodes in the square D . The nodes in the domain are positioned randomly chose from D while the nodes on the boundary is equally spaced. Figure 4.5 is presented the error of numerical integration of f_3 while Figure 4.6 presented the error of numerical integration of f_3 in terms of the log scale respectively.

The exact value of the integration to the function $f_3(x, y)$ is equal to 2.05

Table 4.3 – The error of numerical integration for function f_3 .

Function	Number of scattered points	Numerical integration values	Error
f_3	54	2.07229894505087	$2.22989450508679 \times 10^{-2}$
	504	2.0574447965105	$7.44479651050156 \times 10^{-3}$
	5004	2.05094790837777	$9.47908377769924 \times 10^{-4}$

The results, displayed in the last three Figures (4.7, 4.8 and 4.9), shows that the best-fit is a reasonable representation of the error R_{f_k} .

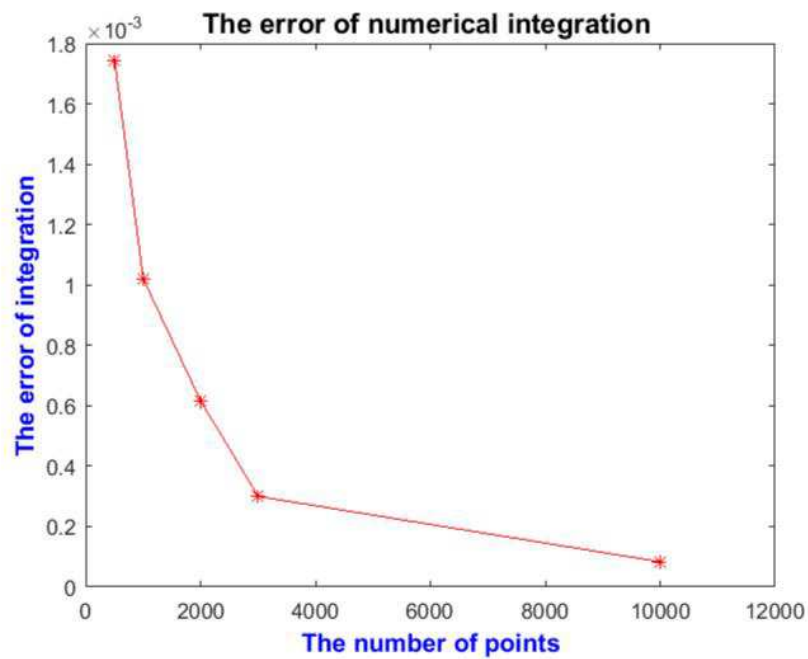


Figure 4.1 – Illustrate the error generated from using cubature formula to approximate the integral of f_1 .

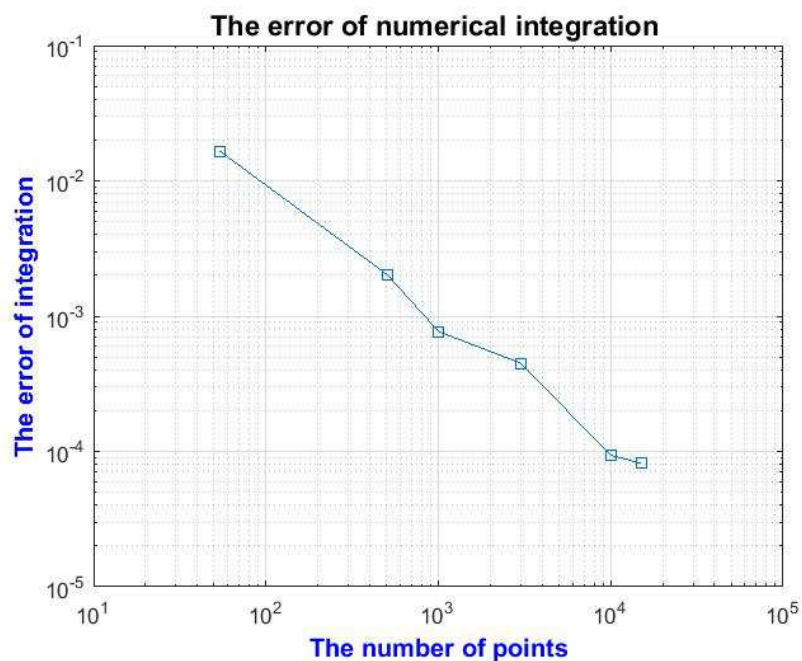


Figure 4.2 – Illustrate the error generated from using cubature formula to approximate the integral of f_1 in the log scale.

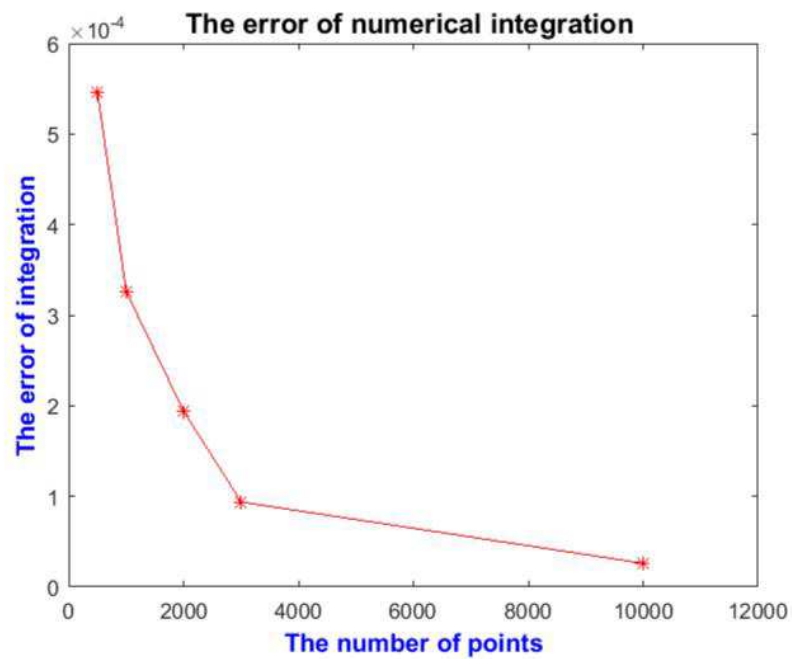


Figure 4.3 – Illustrate the error generated from using cubature formula to approximate the integral of f_2 .

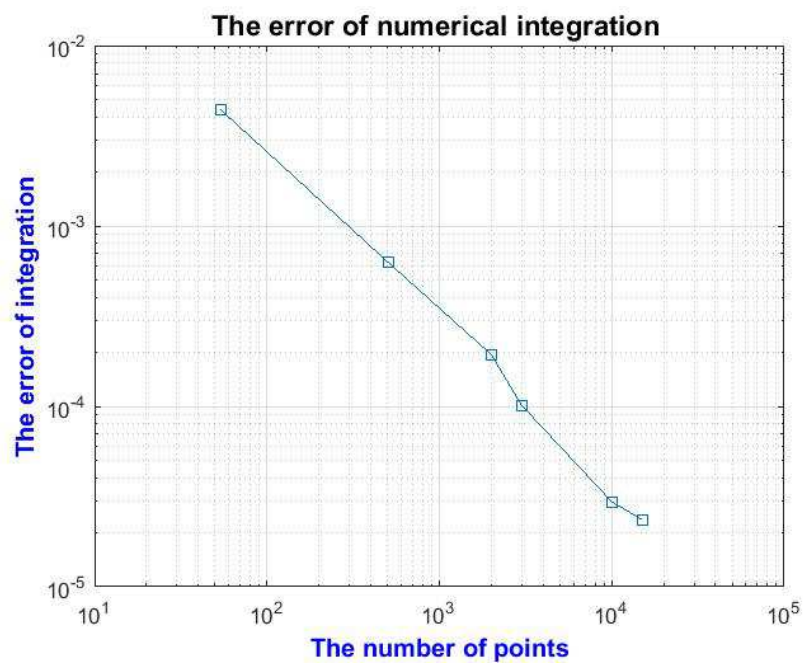


Figure 4.4 – Illustrate the error generated from using cubature formula to approximate the integral of f_2 in the log scale.

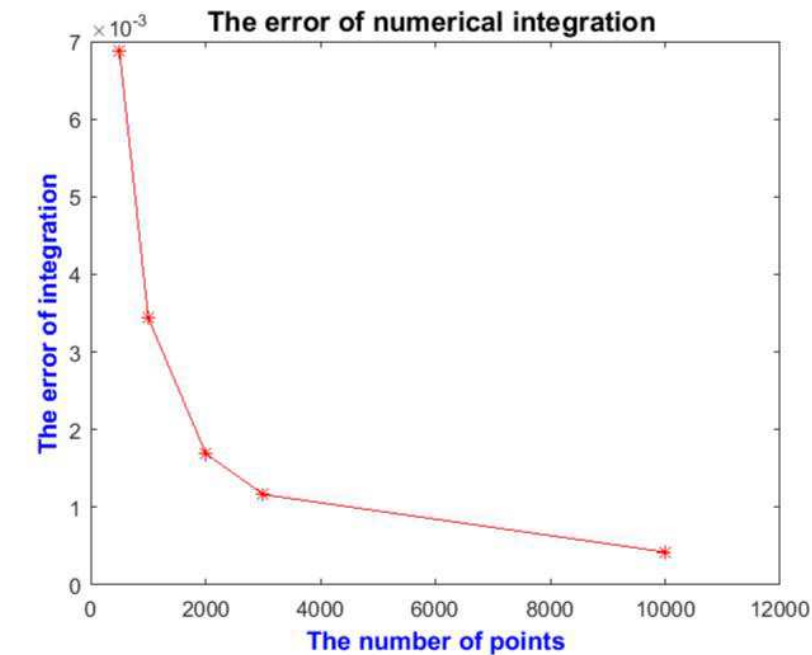


Figure 4.5 – Illustrate the error generated from using cubature formula to approximate the integral of f_3 .

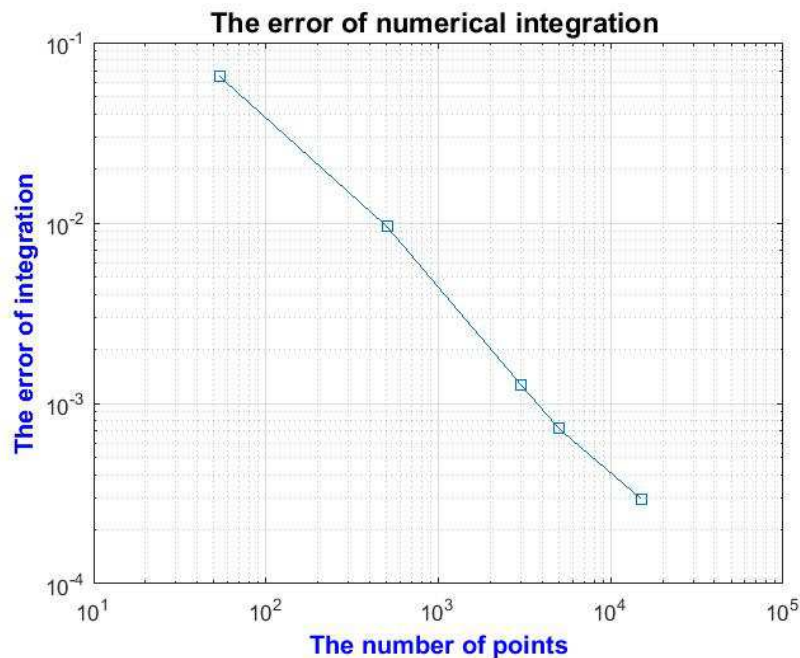


Figure 4.6 – Illustrate the error generated from using cubature formula to approximate the integral of f_3 in the log scale.

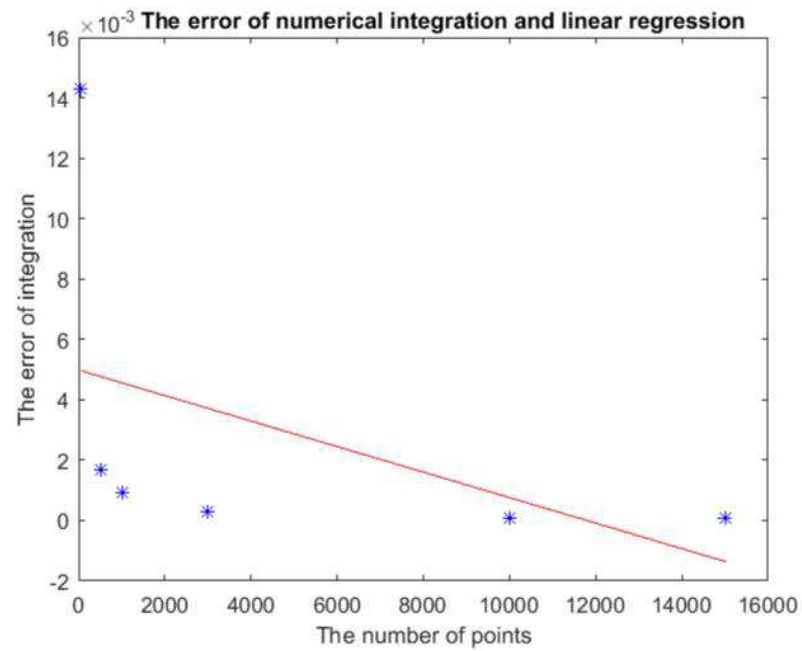


Figure 4.7 – Illustrate the error of numerical integration for function f_1 and linear regression.

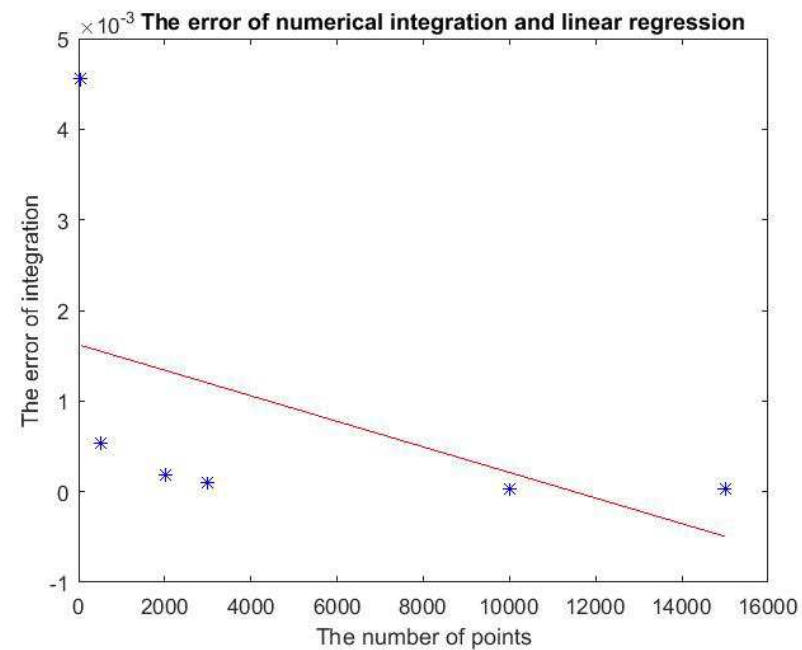


Figure 4.8 – Illustrate the error of numerical integration for function f_2 and linear regression.

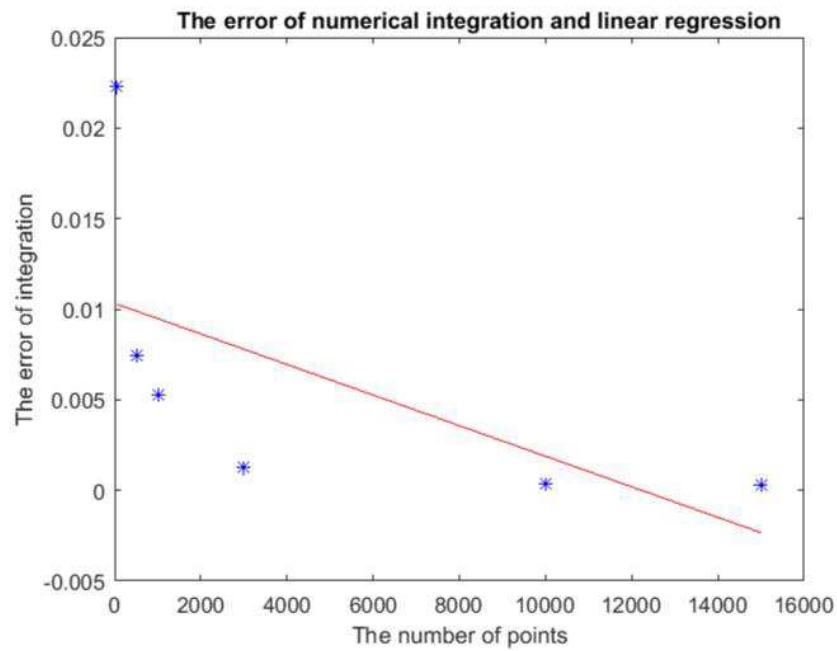


Figure 4.9 – Illustrate the error of numerical integration for function f_3 and linear regression.



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5 New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

This chapter is based on our paper [19] which submitted (2016), however, here, this chapter focuses on the problem of approximating a definite integral of a given function f when, rather than its values at some points, a number of integrals of f over certain hyperplane sections of a d -dimensional hyper-rectangle C_d are only available. We develop several families of integration formulas, all of which are a weighted sum of integrals over some hyperplane sections of C_d , and which contain in a special case of our result multivariate analogues of the midpoint rule, the trapezoidal rule and Simpson's rule. Basic properties of these families are derived, in particular, we show that they satisfy a multivariate version of Hermite-Hadamard inequality. This latter does not require the classical convexity assumption, but it has weakened by a different kind of generalized convexity. As an immediate consequence of this inequality, we derive sharp and explicit error estimates for twice continuously differentiable functions. More precisely, we present explicit expressions of the best constants, which appear in the error estimates for the new multivariate versions of trapezoidal, midpoint, and Hammer's quadrature formulas. It is shown that, as in the univariate case, the constant of the error in the trapezoidal cubature formula is twice as large as that for the midpoint cubature formula, and the constant in the latter is also twice as large as for the new multivariate version of Hammer's quadrature formula. Numerical examples are given comparing these cubature formulas among themselves and with uniform and non-uniform centroidal Voronoi cubatures of the standard form, which use the values of the integrand at certain points.

5.1 Introduction

The central question about which our study revolves is the following one. Assume that f is a function from a hyper-rectangle C_d of dimension greater than one to $\mathbf{R}$, and that the only available data are a number of integrals of f over certain prescribed hyperplane sections of C_d . A relevant question, then, is: how can we get a lower and upper estimate of the exact value of the integral of f over C_d ?

This problem arises in many applications, especially in experimental physics and engineering, where the standard discrete sample values from functions are not available, but only their mean values are accessible. For instance, this data type appears naturally in computer tomography with its many applications in medicine, radiology, geology, amongst others. The mathematical foundation behind these techniques is the work of Johann Radon on the so-called Radon transform [16]. But they also have important applications, especially where the aim is to derive efficient numerical methods for PDEs using the so-called non-conforming Crouzeix–Raviart element. We refer to the recent paper [3] where we have exploited estimators of this type to characterize the enrichment of such element. For more discussion, including potential applications, see [15]. Let us first recall that, under the convexity condition of f , the

one dimensional case has a simple solution. Let f be an integrable real-valued function on the closed real interval $[a, b]$, the midpoint rule for estimating $\int_a^b f(t) dt$ is $M(f) \triangleq f((a+b)/2)$, and the trapezoid rule is $T(f) \triangleq (f(a) + f(b))/2$. An important fundamental property shared by these two rules is the well-known Hermite-Hadamard (double) inequality, which ensures a lower and an upper estimate for the exact value of the integral of any convex function:

$$M(f) \leq \frac{1}{b-a} \int_a^b f(t) dt \leq T(f), \quad (5.1)$$

where the signs of equality being achieved if f is an affine function. The midpoint rule and the trapezoidal rule are the simplest, most well-known and widely used quadrature formulas. They actually served as basic ingredients for constructing more accurate and adaptive formulas by using certain types of their convex combinations or by dividing the interval $[a, b]$ into subintervals and apply these rules to each subinterval (see [17] and [18, § 3.2, §4.2]). For these reasons, these rules together with their fundamental inequality (5.1) have been an effective starting point for several subsequent investigations, see [8, 11]. From the upper and lower bounds (5.1) a better estimate would be to average $M(f)$ and $T(f)$. However, we can do better, in this case, than the simple average of these two rules. Indeed, by simply taking the particular convex combination $(1-\theta)M(f) + \theta T(f)$, with $\theta \in [0, 1]$, we get a more accurate rule. In fact, the approximation obtained in this manner is the very-well known Simpson's rule, and is exact for all polynomials of degree 3. Furthermore, in the error analysis of the rules $M(f)$ and $T(f)$:

$$EM(f) \leq \frac{1}{b-a} \int_a^b f(t) dt - M(f),$$

$$ET(f) \leq T(f) - \frac{1}{b-a} \int_a^b f(t) dt,$$

estimates (5.1) are very useful tools. Indeed, let $(\cdot)^2$ denote the square function $t \mapsto t^2$, and assume that the first derivative of f is a Lipschitz function with a Lipschitz constant $L(f')$ in $[a, b]$, then the following important implications hold:

- (a) The left-hand side of the Hermite-Hadamard inequality implies that for every $f \in C^2[a, b]$ we have

$$|EM(f)| \leq \frac{E M_2^{(1)}(f)}{2} L(f')$$

$$\leq \frac{T \mu^3(a, b)}{6} L(f') \quad (5.2)$$

$$\leq \frac{(b-a)^2}{24} L(f'), \quad (5.3)$$

where equality is attained for all quadratic functions.

- (b) The right-hand side of the Hermite-Hadamard inequality implies that for every $f \in C^2[a, b]$ we have

$$|ET(f)| \leq \frac{E T_2^{(1)}(f)}{2} L(f')$$

$$\leq \frac{T \mu^3(a, b)}{3} L(f') \quad (5.4)$$

$$\leq \frac{(b-a)^2}{12} L(f'), \quad (5.5)$$

where equality is attained for all quadratic functions.

The literature contains a number of variations of these estimations, some statements employing the largest absolute value of the second derivative over the interval $[a, b]$, see, e. g., [11, 20]. One of the interesting aspects of the error estimates (5.3) and (5.5) is that they also characterize the Hermite-Hadamard inequality (5.1), indeed the reverse statements of the above two implications (a) and (b) are valid. In short, equality (5.1) should hold if and only if error estimates (5.3) and (5.5) are satisfied. In fact, they can be easily derived from our multivariate general results given in (5.63) and (5.64).

As for the Hermite-Hadamard inequality for multivariate convex functions, we may refer to [4, 7, 8, 9].

The main objective of this chapter is to establish natural multivariate versions of the midpoint and trapezoidal rules, when the only available data are a number of integrals of f over some hyperplane sections of C_d . In addition, we also give a multivariate version of Simpson's rule in this general setting. Let us mention here that a multivariate version of Simpson's rule also exists for a function f when certain of its *values are only available*, see [21]. We have however observed that cubature formulas, which use the values of the integrand at certain points, give the worst results. Basic properties of our new cubature formulas are derived, in particular, we show that they satisfy a multivariate version of Hermite-Hadamard inequality. This latter does not require the classical convexity assumption, but it has weakened by a different kind of generalized convexity. We shall also see, as we did for the one dimensional case in (5.2) and (5.4) that for such integration formulas, we can also establish a characterization result in terms of sharp error estimates. In addition, we particularly pay attention to the explicit expressions of the best constants, which appear in the error estimates for the new multivariate versions of trapezoidal, midpoint, and Hammer's quadrature formulas [14]. It is shown that, as in the univariate case see (5.2) and (5.4), the constant of the error in the trapezoidal cubature formula is twice as large as that for the midpoint cubature formula, and the constant in the latter is also twice as large as for the new multivariate version of Hammer's quadrature formula.

Let us give a short outline of the chapter. In Section 5.2, we introduce our multivariate version of the trapezoidal rule and present some its important properties. Section 5.3 deals with a multivariate analogue of the midpoint rule, together with some of its properties. In Section 5.4, we introduce and discuss a class of cubature formulas, obtained by averaging the trapezoidal and the midpoint cubature formulas. In particular, it is shown that any cubature formula from this class is always superior to the trapezoidal cubature formula for either componentwise convex or concave functions. In Section 5.5, we generalize Simpson's rule to d dimensions and also provide multivariate versions of perturbed midpoint and trapezoidal rules. Section 5.6 derives sharp error bound with explicit constant for any cubature formula, which is assumed to satisfy an upper or a lower Hermite-Hadamard inequality for any convex functions. In particular, we present explicit expressions of the best constants, which appear in the error estimates for the new multivariate versions of trapezoidal, midpoint, and Hammer's quadrature formulas. In Section 5.7, numerical examples are given comparing these cubature formulas among themselves, and also with uniform and non-uniform centroidal Voronoi cubatures developed in [4]. These latter are of the standard form, since they use a set of numerical values of the integrand at the center of gravity of each element in a subdivision. Finally, concluding remarks, extensions and implications are given in the last section.

Throughout this chapter, we adopt the following notation: Let $\tau_{i1}, \dots, \tau_{d1}$ and $\tau_{i2}, \dots, \tau_{d2}$ be given real numbers such that $\tau_{i1} \leq \tau_{i2}$ for each i . We let C_d denote the d -dimensional hyper-rectangle in $\mathbf{R}^d$ defined by

$$C_d := \{ \mathbf{x} \in (x_1, \dots, x_d), \tau_{i1} \leq x_i \leq \tau_{i2}, i \in 1, \dots, d \}.$$

To simplify notation, we let $L^{\text{tr}}_1, \dots, L^{\text{tr}}_{2d}$ denote the linear functionals

$$L^{\text{tr}}_i(f) = \frac{1}{|F_i|} \int_{F_i} f d\mu, i \in 1, \dots, 2d,$$

$$L^{\text{tr}}_{2d+1}(f) = \frac{1}{|C_d|} \int_{C_d} f(\mathbf{x}) d\mathbf{x}.$$

Here $F_1, \dots, F_{2d}$ are the $2d$ facets of C_d . We will also need a special enumeration of the facets of C_d , for each $j \in 1, \dots, d$, F_j and F_{j+d} are subsets of the hyperplanes $x_j \leq \tau_{j1}$ and $x_j \leq \tau_{j2}$, respectively. Note that F_j and F_{j+d} are two opposite facets of C_d . Here and subsequently, $|C_d|$ and $|F_i|$ denote the d -dimensional volume and the $(d-1)$ -dimensional volume respectively. The following identities hold

$$|C_d| = \prod_{i=1}^d (\tau_{i2} - \tau_{i1})$$

$$|F_j| = |F_{j+d}| = \prod_{i \neq j} (\tau_{i2} - \tau_{i1}) = \frac{|C_d|}{\tau_{j2} - \tau_{j1}}.$$

For any $i \in 1, \dots, d$, we write $C_{d,i}$ for the $(d-1)$ -dimensional hyper-rectangle in $\mathbf{R}^{d-1}$ defined by

$$C_{d,i} := \{ \mathbf{u} \in (u_1, \dots, u_{i-1}, u_{i+1}, \dots, u_d), \tau_{i1} \leq u_j \leq \tau_{i2}, j \in 1, \dots, d, j \neq i \}.$$

Let us now introduce the definition of componentwise convexity, which is a weaker version of the classical convexity, see e.g., [12, 13]. This is made precise by the following:

Definition 5.1.1 A function $f : C_d \rightarrow \mathbf{R}$ is called *componentwise convex* if it is convex in each coordinate when the other coordinates are held fixed, that is, for each $i \in 1, \dots, d$, and for arbitrarily fixed $\mathbf{x}_{j2} \in [\tau_{j1}, \tau_{j2}]$ ($j \neq i$), the real function $\tilde{f} : [\tau_{i1}, \tau_{i2}] \rightarrow \mathbf{R}$, defined by

$$\tilde{f}(x_i) := f(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_d)$$

is convex.

Let us note that classical convexity implies componentwise convexity, but the converse is not necessarily true. Indeed, let $d \geq 2$ and let the function $f : [0, 1]^d \rightarrow [0, 1]$ defined by

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

$f(\mathbf{x}) \in Q^d_{i \in 1} x_i^2$. Since

$$\frac{\partial^2 f(\mathbf{x})}{\partial x_i^2} \in 2 \prod_{j=1, j \neq i}^d x_j^2,$$

then f is componentwise convex but f is not convex on $[0,1]^d$. Indeed, if $\mathbf{x} \in (0, x_2, \dots, x_d)$, $\mathbf{y} \in (x_1, 0, x_3, \dots, x_d) \in (0, 1)^d$ and $\theta \in (0, 1)$, we have:

$$f(\theta \mathbf{x} \dot{\wedge} (1-\theta) \mathbf{y}) \in \theta^2 (1-\theta)^2 \prod_{i \in 1}^d x_i^2 \text{ and } \theta f(\mathbf{x}) \dot{\wedge} (1-\theta) f(\mathbf{y}) \in 0.$$

Thus, for all $\theta \in (0,1)$ we have $f(\theta \mathbf{x} \dot{\wedge} (1-\theta) \mathbf{y}) \dot{\neq} \theta f(\mathbf{x}) \dot{\wedge} (1-\theta) f(\mathbf{y})$, which shows that f is not convex on $[0,1]^d$. It is obvious that, in the particular case $d \in 1$, the two notions of convexity coincide.

5.2 A multivariate version of the trapezoidal rule

The goal of this section is to introduce a new family of a multivariate version of the well-known trapezoidal rule. We also establish multivariate analogues of the right hand side of the Hermite-Hadamard inequality. We first define a special class of linear functionals, for each $i \in 1, \dots, d$, we set

$$E_i^{\text{tr}}(f) := L_{2d \dot{\wedge} 1}^{\text{tr}}(f) - Q_i^{\text{tr}}(f), \quad (5.6)$$

where

$$Q_i^{\text{tr}}(f) \in \frac{1}{2} L_{i \dot{\wedge} 1}^{\text{tr}}(f) \dot{\wedge} L_{i \dot{\wedge} d}^{\text{tr}}(f) \quad (5.7)$$

$$\in \frac{1}{2} \left(\frac{1}{\mu} \int_{F_i} f d\mathcal{B}_i \dot{\wedge} \frac{1}{\mu} \int_{F_i \dot{\wedge} d} f d\mathcal{B}_i \right). \quad (5.8)$$

Functional E_i^{tr} can be viewed as the approximation error when approximating $\int_{C^1[d]} f(\mathbf{x}) d\mathbf{x}$ with $\frac{1}{2} \left(\frac{1}{\mu} \int_{F_i} f d\mathcal{B}_i \dot{\wedge} \frac{1}{\mu} \int_{F_i \dot{\wedge} d} f d\mathcal{B}_i \right)$.

The main observation we first need to make is the following Lemma:

Lemma 5.2.1 For each $i \in 1, \dots, d$, the approximation error E_i^{tr} as defined in equation (5.6) vanishes for all affine functions.

Proof Since all functionals $L_{i \dot{\wedge} i}^{\text{tr}}, i \in 1, \dots, 2d \dot{\wedge} 1$, preserve constants, then obviously E_i^{tr} necessarily vanishes for all constants. Since E_i^{tr} is linear, it remains to show that, for all $j \in 1, \dots, d$,

we have $E_l^{\text{tr}}(x_j) \neq 0$. Now, we can immediately obtain the following identities:

$$\begin{aligned} L_{i,j}^{\text{tr}}(x_j) &\neq \frac{\sum_{j_1=1}^2 \sum_{j_2=1}^2 \sum_{j_3=1}^2 \sum_{j_4=1}^2 \pm_{ij}^{\epsilon}}{2^d}, \quad i, j \in 1, \dots, d, \\ L_{i,j}^{\text{tr}}(x_j) &\neq \frac{\sum_{j_1=1}^2 \sum_{j_2=1}^2 \sum_{j_3=1}^2 \pm_{ij}^{\epsilon}}{2^d}, \quad i, j \in 1, \dots, d, \\ L_{2d+1}^{\text{tr}}(x_j) &\neq \frac{\sum_{j_1=1}^2 \sum_{j_2=1}^2 \pm_{ij}^{\epsilon}}{2^d}, \quad j \in 1, \dots, d. \end{aligned}$$

Hence it follows that

$$L_{2d+1}^{\text{tr}}(x_j) \neq \frac{L_{i,j}^{\text{tr}}(x_j) \neq L_{i,j}^{\text{tr}}(x_j)}{2}, \quad i, j \in 1, \dots, d. \quad (5.9)$$

or equivalently

$$E_l^{\text{tr}}(x_j) \neq 0, \quad i, j \in 1, \dots, d. \quad (5.10)$$

We can immediately conclude that for any $i \in 1, \dots, d$, the approximation error E_l^{tr} vanishes for all affine functions. ■

We are now ready to define our multivariate version of the trapezoidal rule. To this end, let us introduce the following error functional:

$$E^{\text{tr}}(f) := L_{2d+1}^{\text{tr}}(f) - Q^{\text{tr}}(f), \quad (5.11)$$

with

$$\frac{1}{x} = \sum_{i=1}^d \frac{1}{x_i} \quad (5.12)$$

where $Q_l^{\text{tr}}(f)$ is defined by (5.7). We observe that for the one-dimensional case, $d \in 1$, the trapezoidal cubature formula $Q^{\text{tr}}(f)$ reduces to the trapezoidal rule. Moreover, as in the one-dimensional case, the following theorem shows that the multivariate version (5.12) also enjoys a property of affine functions vanishing similar to the trapezoidal rule.

Theorem 5.2.2 *The approximation error E^{tr} of the trapezoidal cubature formula as defined in equation (5.11) vanishes for all affine functions.*

Proof Indeed, just observe that the approximation error of the the trapezoidal cubature

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

formula (5.11) can simply be written as

$$E_i^{\text{tr}}(f) = \int_{C_d} L_{2d}^{\text{tr}}(f) \cdot Q_i^{\text{tr}}(f) - \frac{1}{d} \sum_{i \in I} L_{2d}^{\text{tr}}(f) \cdot Q_i^{\text{tr}}(f) \\ = \frac{1}{d} \sum_{i \in I} X_d E_i^{\text{tr}}(f),$$

where $E_i^{\text{tr}}(f)$ is the error functional define in Lemma 5.2.1. We now apply the latter, which asserts that, for any $i \in 1, \dots, d$, E_i^{tr} vanishes for all affine functions, then our desired result follows immediately. ■

We now establish our multivariate version of right hand side of Hermite-Hadamard's inequality (5.1) for componentwise convex functions.

Theorem 5.2.3 *Let f be a componentwise convex on C_d . Then*

$$\int_{C_d} f(x) dx \cdot Q^{\text{tr}}(f) = \frac{1}{d} \sum_{i \in I} \int_{C_{d,i}} f(x) dx \cdot Q_i^{\text{tr}}(f). \quad (5.13)$$

Proof Fix $x \in (x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_d)$ and define $f_i: [-i_1, -i_2] \rightarrow \mathbb{R}$, $f_i(t) \in f(x_1, \dots, x_{i-1}, t, x_{i+1}, \dots, x_d)$. But, since by assumption f is componentwise convex on C_d , then it follows that the function f_i is convex on $[-i_1, -i_2]$ for all $(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d) \in C_{d,i}$. Then by Hermite-Hadamard inequality (5.1) we get

$$\int_{-i_2}^{-i_1} f_i(t) dt \cdot \frac{1}{-i_2 - (-i_1)} \leq \frac{f_i(-i_1) + f_i(-i_2)}{2} \\ \int_{-i_2}^{-i_1} f_i(t) dt \cdot \frac{1}{-i_2 - (-i_1)} \leq \frac{f_i(-i_1) + f_i(-i_2)}{2}, \quad (5.14)$$

or, equivalently, for every $(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d) \in C_{d,i}$, we have

$$\int_{-i_2}^{-i_1} f(x_1, \dots, x_{i-1}, t, x_{i+1}, \dots, x_d) dt \cdot \frac{-i_2 - (-i_1)}{2} \\ \leq (f(x_1, \dots, x_{i-1}, -i_1, x_{i+1}, \dots, x_d) + f(x_1, \dots, x_{i-1}, -i_2, x_{i+1}, \dots, x_d)).$$

Integrating this inequality on $C_{d,i}$, and using Fubini's theorem we immediately arrive at

$$\int_{C_d} f(x) dx \cdot \frac{1}{d} \leq \frac{1}{2} \sum_{i \in I} \int_{C_{d,i}} L_{2d}^{\text{tr}}(f) \cdot L_{2d}^{\text{tr}}(f) dx. \quad (5.15)$$

Now, summing these inequalities over $1 \leq i \leq d$, then divide by d yields the assertion. This completes the proof. ■

5.3 A multivariate version of the midpoint rule

We now define our multivariate version of the midpoint rule. To this end, we need the following linear functionals

$$Q_i^{\text{mid}}(f) = \frac{1}{|M_i|} \int_{M_i} f d\beta_d, \quad i \in 1, \dots, d, \quad (5.16)$$

where, for each i , M_i is the hyperplane section of C_d defined by

$$M_i = \{x \in C_d, x_i = \frac{1}{2}\}. \quad (5.17)$$

Setting

$$E^{\text{mid}}(f) = L^{\text{tr}}_{2d \times 1}(f) - Q^{\text{mid}}(f), \quad (5.18)$$

with

$$Q^{\text{mid}}(f) = \frac{1}{d} \sum_{i=1}^d Q_i^{\text{mid}}(f) \quad (5.19)$$

where $Q_i^{\text{mid}}(f)$ is defined by (5.16). It is easy to check that for the one-dimensional case, $d = 1$, the midpoint cubature formula (5.19) reduces to the midpoint rule. Moreover, as in the one-dimensional case, it satisfies:

Theorem 5.3.1 *The approximation error E^{mid} of the midpoint cubature formula as defined in equation (5.18) vanishes for all affine functions.*

Proof An alternative expression of the approximation error E^{mid} is

$$E^{\text{mid}}(f) = L^{\text{tr}}_{2d \times 1}(f) - \frac{1}{d} \sum_{i=1}^d Q_i^{\text{mid}}(f), \quad (5.20)$$

$$= \frac{1}{d} \sum_{i=1}^d E_i^{\text{mid}}(f), \quad (5.21)$$

where $E_i^{\text{mid}}(f)$ is the error in approximating $L^{\text{tr}}_{2d \times 1}(f)$ with $Q_i^{\text{mid}}(f)$. As can be seen from (5.21), it will now suffice to show that $E_i^{\text{mid}}(f)$ vanishes for all affine functions. In order to prove this

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

assertion, note that the following identities hold, for every $i \in 1, \dots, d$,

$$L_{2d-1}^{\text{tr}}(x_j) \in Q_i^{\text{mid}}(x_j) \in \frac{j^1 - j^2}{2}, j \in 1, \dots, d, \quad (5.22)$$

and for every $c \in \mathbf{R}$, we have

$$L_{2d-1}^{\text{tr}}(c) \in Q_i^{\text{mid}}(c) \in c. \quad (5.23)$$

Hence, combining (5.22) and (5.23), we get, for every affine function f ,

$$L_{2d-1}^{\text{tr}}(f) \in Q_i^{\text{mid}}(f), (i \in 1, \dots, d), \quad (5.24)$$

which together with (5.20) implies that the desired result holds. ■

We now present our multivariate version of left hand side of Hermite-Hadamard's inequality (5.1) for componentwise convex functions.

Theorem 5.3.2 *Let f be a componentwise convex on C_d . Then*

$$\frac{1}{x} \frac{d}{1} \frac{1}{\mathbf{Z}} \frac{1}{M_i f d^{3/4}} \frac{1}{j} \frac{1}{C^1 d} \frac{1}{\mathbf{Z}} \frac{1}{C_d} f(\mathbf{x}) d \mathbf{x}. \quad (5.25)$$

Proof Fix $\mathbf{x} \in (x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_d)$ and define $f_i: [i-1, i+2] \rightarrow \mathbf{R}$, $f_i(t) \in f(x_1, \dots, x_{i-1}, t, x_{i+1}, \dots, x_d)$. According to the fact that f is componentwise convex on C_d , it follows that the function f_i is convex on $[i-1, i+2]$ for all $(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d) \in C_{d-i}$. Then by Hadamard's inequality (5.1) we get

$$(i+2 - i-1) f_i \left(\frac{i-1 + i+2}{2} \right) \leq \int_{i-1}^{i+2} f_i(t) dt \quad (5.26)$$

or, equivalently, for every $(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d) \in C_{d-i}$, we have

$$(i+2 - i-1) f(x_1, \dots, x_{i-1}, (i-1 + i+2)/2, x_{i+1}, \dots, x_d) \leq \int_{i-1}^{i+2} f(x_1, \dots, x_{i-1}, t, x_{i+1}, \dots, x_d) dt.$$

Integrating this inequality on C_{d-i} , and using Fubini's theorem we immediately arrive at

$$Q_i^{\text{mid}}(f) \leq \frac{1}{\mathbf{Z}} \frac{1}{C_d} f(\mathbf{x}) d \mathbf{x}, (i \in 1, \dots, d). \quad (5.27)$$

Now, summing these inequalities over $1 \leq i \leq d$, then divide by d yields the assertion. This completes the proof. ■

5.4 Average cubature formulas

In this section, we consider a class of cubature formulas that can be expressed as convex combinations of the trapezoidal cubature (5.12) and the midpoint cubature formulas (5.19), that is, for any $\theta \in [0, 1]$, we have

$$\frac{1}{d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} \approx \theta Q^{\text{mid}}(f) + (1 - \theta) Q^{\text{tr}}(f). \quad (5.28)$$

The idea is to choose θ so that the resulting cubature formula approximates from above, or from below, the integral of every componentwise convex function f on C_d . Note that family (5.28) gives the trapezoidal cubature formula when $\theta \in 0$ and the midpoint cubature formula when $\theta \in 1$. The following lemma can be easily deduced from a general result in [8, Theorem 4.1].

Lemma 5.4.1 *For every convex function $f : [a, b] \rightarrow \mathbf{R}$ and every $\theta \in [0, 1/2]$ the following inequality holds true*

$$\frac{1}{b-a} \int_a^b f(t) dt \leq \theta f((a+b)/2) + (1 - \theta)(f(a) + f(b))/2. \quad (5.29)$$

As a function of θ , the right-hand side of (5.29) is non-increasing on $[0, 1]$. Moreover, for every $\theta \in [1/2, 1]$, there exists a convex function f for which (5.29) is false.

As extensions of Theorems 5.2.3 and 5.3.2 we obtain the following result:

Theorem 5.4.2 *Let Q^{tr} and Q^{mid} be the cubature formulas given respectively by (5.12) and (5.19). Then, for every componentwise convex function f on C_d , and $\theta \in [0, 1/2]$ we have*

$$\frac{1}{d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} \leq \theta Q^{\text{mid}}(f) + (1 - \theta) Q^{\text{tr}}(f). \quad (5.30)$$

As a function of θ , the right-hand side of (5.30) is non-increasing on $[0, 1]$. Moreover, for every $\theta \in [1/2, 1]$, there exists a componentwise convex function f for which (5.30) is false.

Proof Fix $\mathbf{x} \in (x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_d)$. Since, f is componentwise convex on C_d then $f_i : [x_{i-1}, x_{i+1}] \rightarrow \mathbf{R}$, $f_i(t) \in f(x_1, \dots, x_{i-1}, t, x_{i+1}, \dots, x_d)$, is convex on $[x_{i-1}, x_{i+1}]$ for all $(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d) \in C_d$. Hence by Lemma 5.4.1 we get, for any $\theta \in [0, 1/2]$,

$$\frac{1}{x_{i+1} - x_{i-1}} \int_{x_{i-1}}^{x_{i+1}} f_i(t) dt \leq \theta f_i((x_{i-1} + x_{i+1})/2) + (1 - \theta)(f_i(x_{i-1}) + f_i(x_{i+1})). \quad (5.31)$$

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

Integrating this inequality on C_d , and using Fubini's theorem we immediately arrive at

$$\frac{1}{j} \int_{C_d} f(\mathbf{x}) d\mathbf{x} \cdot Q_i^{\text{mid}}(f) \leq (1 - \theta) Q_i^{\text{tr}}(f), \quad (i \in 1, \dots, d) \quad (5.32)$$

Finally, summing these inequalities over $1 \leq i \leq d$, and then dividing both sides by d yields the required inequality. By standard considerations, the rest of the proof is easy using another application of Lemma 5.4.1. ■

We are now in a position to show that the midpoint cubature Q^{mid} and more generally the average cubature formulas $Q_\theta(f) \leq Q^{\text{mid}}(f) \leq (1 - \theta) Q^{\text{tr}}(f)$, $\theta \in [0, 1]$ are always superior to Q^{tr} if f is componentwise convex or concave on C_d . An improvement of this result will be obtained for differentiable functions with Lipschitz continuous gradients, see Section 5.6. In one dimension, inequality (5.33) is due to Hammer [14].

Corollary 5.4.3 *Let f be a function either componentwise concave or convex on C_d . Then*

$$\frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} \leq Q^{\text{mid}}(f) \leq Q^{\text{tr}}(f) \leq \frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x}. \quad (5.33)$$

More generally, for any $\theta \in [0, 1]$, we have

$$\frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} \leq Q_\theta(f) \leq Q^{\text{tr}}(f) \leq \frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x}. \quad (5.34)$$

Proof We begin with the first statement. We only give the proof in the case when f is componentwise convex, the case of the concavity can be obtained similarly by replacing f by $-f$, so we omit the details. To this end, we will prove the following equivalent inequalities

$$0 \leq \frac{1}{j} \int_{C_d} f(\mathbf{x}) d\mathbf{x} - Q^{\text{mid}}(f) \leq Q^{\text{tr}}(f) - \frac{1}{j} \int_{C_d} f(\mathbf{x}) d\mathbf{x}. \quad (5.35)$$

The left-hand inequality follows directly from Theorem 5.3.2. For the right-hand inequality it suffices to observe that (5.35) is equivalent to

$$\frac{1}{j} \int_{C_d} f(\mathbf{x}) d\mathbf{x} \leq \frac{1}{j} Q^{\text{mid}}(f) \leq \frac{1}{j} Q^{\text{tr}}(f), \quad (5.36)$$

which is satisfied by choosing $\theta \in \frac{1}{2}$ and applying Theorem 5.4.2. As a consequence of (5.33), we may now prove the general inequality (5.34). Indeed, an easy calculation shows that the following estimate holds:

$$\begin{aligned} \frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} - Q_\theta(f) &= \frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} - Q^{\text{mid}}(f) - \\ &= \frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} - Q^{\text{tr}}(f) + Q^{\text{tr}}(f) - Q_\theta(f) \\ &= \frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} - Q^{\text{tr}}(f) + \theta \int_{C_d} f(\mathbf{x}) d\mathbf{x} - \theta Q^{\text{tr}}(f) \\ &= \theta \left(\frac{1}{C_d} \int_{C_d} f(\mathbf{x}) d\mathbf{x} - Q^{\text{tr}}(f) \right) \leq 0 \end{aligned}$$

Thus, combining the above inequality and (5.33), we obtain the required general inequality.

■

5.5 A multivariate version of perturbed midpoint, trapezoidal, and Simpson's rule

We shall now generalize Simpson's rule to d dimensions. We also provide multivariate versions of perturbed midpoint and trapezoidal rules. Recall that, for any $i \in 1, \dots, d$, M_i is the hyper-plane section defined as in (5.17). Here, we continue to denote by Q_i^{tr} and Q_i^{mid} the functionals given respectively by (5.7) and (5.16). Throughout the rest of this section, for nonnegative integer n , P_n will denote the vector space of polynomials on C_d with real coefficients of degree at most n . We start with the following key remark.

Remark 5.5.1 Let us also observe the following surprising result. By Theorem 5.2.2 and 5.3.1, we know that the trapezoidal and midpoint cubature formulas are each only exact for linear functions. However, it can be easily verified that, for each $i \in 1, \dots, d$, the approximation errors E_i^{tr} and E_i^{mid} given respectively by (5.6) and (5.18) vanish on the space

$$Q := P_1 \otimes \left(\bigotimes_{j \in 1, \dots, d, j \neq i} P_{\infty} \right). \quad (5.37)$$

Moreover, if we denote by

$$I = \frac{1}{d!} \int_{C_d} f(x) dx = \frac{1}{d!} \int_{C_d} f(x) dx, \quad Q = \frac{1}{d!} \int_{C_d} f(x) dx,$$

then the following key identities hold, for any $\alpha_j \in \mathbb{N}$, $j \in 1, \dots, d$, $j \neq i$ and $\alpha_i \in 0, 1, 2, 3$,

$$Q_i^{\text{tr}} \left(\prod_{j \in 1, \dots, d, j \neq i} x_j^{\alpha_j} \right) = \frac{1}{d!} \int_{C_d} \prod_{j \in 1, \dots, d, j \neq i} x_j^{\alpha_j} dx, \quad (5.38)$$

$$Q_i^{\text{mid}} \left(\prod_{j \in 1, \dots, d, j \neq i} x_j^{\alpha_j} \right) = \frac{1}{d!} \int_{C_d} \prod_{j \in 1, \dots, d, j \neq i} x_j^{\alpha_j} dx, \quad (5.39)$$

$$\frac{1}{d!} \int_{C_d} \prod_{j \in 1, \dots, d, j \neq i} x_j^{\alpha_j} dx = \frac{1}{d!} \int_{C_d} \prod_{j \in 1, \dots, d, j \neq i} x_j^{\alpha_j} dx = \frac{1}{d!} \int_{C_d} \prod_{j \in 1, \dots, d, j \neq i} x_j^{\alpha_j} dx, \quad (5.40)$$

It should be mentioned that the requirements $\alpha_j \in 0, 1, 2, 3$ concern only equality (5.40).

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

Let us now define, for each $i \in 1, \dots, d$, the integration formula.

$$\frac{1}{j} \int_{j}^{j+1} f(x) dx \approx \frac{1}{3} Q_i^{\text{tr}}(f) + \frac{2}{3} Q_i^{\text{mid}}(f) + E_i^{\text{Sim}}(f) \quad (5.41)$$

$$E_i^{\text{Sim}}(f). \quad (5.42)$$

For the cubature formula (5.41), the following result holds.

Lemma 5.5.2 For each $i \in 1, \dots, d$, the approximation error E_i^{Sim} as defined in (5.42) vanishes for all functions belonging to P_3 .

Proof Let us first observe that the approximation error E_i^{Sim} can be written as

$$E_i^{\text{Sim}} = \frac{1}{3} E_i^{\text{tr}} + \frac{2}{3} E_i^{\text{mid}}, \quad i \in 1, \dots, d, \quad (5.43)$$

where E_i^{tr} and E_i^{mid} are respectively defined by (5.6) and (5.18). Remark 5.5.1 tells us that, for each $i \in 1, \dots, d$, these latter vanish on the space Q , where Q is defined by (5.37). Then, since E_i^{Sim} is a convex combination of these two approximation errors, it consequently vanishes on the same space. Hence, E_i^{Sim} vanishes identically for any $f \in P_3$ provided that

$$E_i^{\text{Sim}} = \sum_{j \in 1}^d x_j^{\otimes j} \approx 0,$$

for any $\otimes j \in \mathbf{N}$, $j \in 1, \dots, d$, $j \leq 3$, such that $\sum_{j \in 1}^d \otimes j \leq 3$. This required equality now follows from identity (5.40). ■

Let us now define the integration formula.

$$\frac{1}{j} \int_{j}^{j+1} f(x) dx \approx \frac{2}{3} Q^{\text{mid}}(f) + \frac{1}{3} Q^{\text{tr}}(f) + E^{\text{Sim}}(f), \quad (5.44)$$

where Q^{tr} and Q^{mid} are the cubature formulas given respectively by (5.12) and (5.19). Recall that Simpson's rule can be expressed on the interval $[a, b]$ as:

$$\frac{b-a}{6} \int_a^b f(t) dt \approx \frac{2}{6} f\left(\frac{a+b}{2}\right) + \frac{1}{6} f(a) + \frac{1}{6} f(b) = E^{\text{Sim}}(f). \quad (5.45)$$

Hence, the cubature formula (5.44) appears as a natural extension to higher dimensions of the classical Simpson's rule. For the Simpson cubature formula (5.44), the following result holds.

5.5. A multivariate version of perturbed midpoint, trapezoidal, and Simpson's rule

Theorem 5.5.3 Let Q^{tr} and Q^{mid} be the cubature formulas given respectively by (5.12) and (5.19). Then, the approximation error E^{Sim} as defined in (5.44) vanishes for all functions belonging to P_3 .

Proof Indeed, it is obvious that the approximation error E^{Sim} can be expressed as follows:

$$E^{Sim}(f) = \frac{1}{d} \sum_{i \in I} E_i^{Sim}(f),$$

Hence, it remains to apply Lemma 5.5.2 to get the required result. ■

Let us also introduce another class of cubature formulas via

$$\frac{1}{j!} \int_{\mathcal{C}_d} f(\mathbf{x}) d\mathbf{x} \approx Q^{mid}(f) + Q^{mper}(f) + E^{mper}(f), \quad (5.46)$$

where Q^{mid} is the cubature formula defined by (5.25) and

$$Q^{mper}(f) := \frac{1}{d} \sum_{\mathbf{x}} \frac{(-1)^{2j-1}}{(2j-1)!} \int_{\mathcal{C}_d} f(\mathbf{x}) d\mathbf{x}. \quad (5.47)$$

Atkinson [2] defined the corrected or perturbed midpoint rule on the interval $[a, b]$ by

$$\frac{1}{b-a} \int_a^b f(t) dt \approx \frac{f(a) + f(b)}{2} + \frac{f'(b) - f'(a)}{24} + E^{mper}(f), \quad (5.48)$$

and so the cubature formula (5.46) is a natural extension of the perturbed midpoint rule in higher dimensions.

It also holds that the cubature formula (5.46) satisfies the following exactness condition.

Theorem 5.5.4 The approximation error of the perturbed midpoint cubature formula E^{mper} vanishes for all functions belonging to P_2 .

Proof The proof simply follows from Remark 5.5.1. First, let us observe that

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

$$\begin{aligned} E^{\text{mper}}(f) &\in \frac{1}{d!} \int_{C_d} f(x) dx \in Q^{\text{mper}}(f) \\ &\in \frac{1}{d!} \int_{C_d} f(x) dx \in Q^{\text{mid}}(f) \prod_{i=1}^d Q^{\text{mper}}(f) \\ &\in \frac{1}{d!} \int_{C_d} f(x) dx \in Q^{\text{mid}}(f) \prod_{i=1}^d Q^{\text{mper}}(f) \\ &\in \frac{1}{d!} \int_{C_d} f(x) dx \in Q^{\text{mid}}(f) \prod_{i=1}^d Q^{\text{mper}}(f) \end{aligned}$$

To show the desired result, it suffices to show that

$$E^{\text{mper}}(f) \in 0.$$

for any $0 \leq j \leq 2, j \in 1, \dots, d$, such that $\prod_{j \in 1}^d j = 2$.
Now, since we have the following identities

$$\prod_{j \in 1}^d j = 0, \quad \text{otherwise,}$$

and

$$\frac{(-1)^{2j} (j-1)!}{24 C_d} \int_{C_d} f(x) dx \in Q^{\text{mid}}(f) \prod_{i=1}^d Q^{\text{mper}}(f) \quad (5.50)$$

for any $j \geq 2, j \in 1, \dots, d, j \in 1, \dots, d, j \in 1, \dots, d$, such that $\prod_{j \in 1}^d j = 2$. Then, the desired result follows immediately.

We now turn to another perturbed version of the trapezoidal cubature formula:

$$\frac{1}{d!} \int_{C_d} f(x) dx \in Q^{\text{tr}}(f) \in Q^{\text{tper}}(f) \in E^{\text{tper}}(f), \quad (5.51)$$

where Q^{tr} is the cubature formulas defined by (5.13) and Q^{tper} defined as follows

$$\int_{C_d} f(x) dx$$

$$Q^{\text{tper}}(f) \in \frac{1}{d!} \int_{C_d} f(x) dx \in Q^{\text{tper}}(f) \in E^{\text{tper}}(f) \quad (5.52)$$

In this case we have the following result:

124

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

Our characterization of an integration formula, which admits an upper or a lower Hermite-Hadamard inequality, can be phrased as follows:

Theorem 5.6.2 Let $H_i, i \in 1, \dots, n$, be some given hyperplane sections with positive measures of the d -dimensional hyper-rectangle C_d , and let $l_i, i \in 1, \dots, n$, be n positive real numbers. Define the integration formula via

$$\frac{1}{j} \int_{C_d} f(x) dx \approx \sum_{i=1}^n \frac{l_i}{j} \int_{H_i} f d\mu_i,$$

and let $\alpha \in \{1, 1\}$. Then, the two following statements are equivalent

(i) For every convex function $g \in C^{1,1}(C_d)$, we have

$$\frac{1}{j} \int_{C_d} g(x) dx \geq 0. \quad (5.57)$$

(ii) For every $f \in C^{1,1}(C_d)$ with $L(f)$ -Lipschitz gradient, we have

$$\frac{1}{j} \int_{C_d} f(x) dx \geq \frac{1}{j} \int_{C_d} f(x) dx - \frac{L(f)}{2}. \quad (5.58)$$

Equality is attained for all functions of the form

$$f(x) = a(x) + c k^2, \quad (5.59)$$

where $c \in \mathbb{R}$ and $a(x)$ is any affine function.

Proof First we prove (i) implies (ii). Take f to be any continuous function from $C^{1,1}(C_d)$ with Lipschitz constant $L(f)$, and define the two following functions

$$g(x) = \frac{L(f)}{2} k^2 + f(x).$$

According to [7, proposition 2.2], we know that both of these functions are convex and clearly belong to $C^{1,1}(C_d)$. Hence, by applying (5.57) to g , we immediately deduce

$$\frac{1}{j} \int_{C_d} g(x) dx \geq 0,$$

or equivalently, by using the linearity of E ,

$$\frac{1}{j} \int_{C_d} g(x) dx \geq \frac{L(f)}{2} + \frac{1}{j} \int_{C_d} f(x) dx.$$

This is equivalent to the desired result (5.58).

For the statement on the occurrence of equality, it is enough to note that if E satisfies (5.57) for

all convex functions from $C^{1,1}(C_d)$ then it must vanish for affine functions. Let us now prove that (ii) implies (i). It clearly follows from (5.58) that

$${}_{3/4}E_{\mathbf{k},\mathbf{k}^2}, 0, \quad (5.60)$$

and that, for any $f \in C^{1,1}(C_d)$,

$$\frac{2}{3} E_{\text{k.k}} \frac{L(rf)}{2} \rightarrow 0. \quad (5.61)$$

Now, let us take an arbitrary convex function $g \in C^{1,1}(C_d)$, and define

$$f : \mathbb{A}^1_{\mathbb{F}_q} \rightarrow \mathbb{A}^1_{\mathbb{F}_q}$$

Then, by [7, proposition 2.2], we have

$$f_2 \in C^{1,1}(C_d) \text{ with } L(rf) \cdot L(rg). \quad (5.62)$$

Furthermore, since

$$g \propto \frac{L(r_g)}{2} k \cdot k^2 \mid f,$$

we obviously have

$$g \approx \frac{\mu L(rf)}{k^2} + f \frac{\mu L(rg)}{k^2} + \frac{L(rf)}{2},$$

and hence we arrive at

$$\frac{2}{3}E \frac{L(rf)}{2} \frac{L(rg)}{2} \frac{L(rf)}{2}$$

Finally, (5.60), (5.61) together with (5.62) yield that (i) is valid. This shows the equivalence between these two statements. ■

We will let $\mathbf{c}^\sharp$ denote the center of gravity of C_d defined by $\mathbf{c}^\sharp \in \bigcap_{i=1}^d \frac{A_{i-1}}{2}, i \in 1 \dots, d$. We may now combine Theorems 5.2.3, 5.3.2, 5.4.2, 5.5.3, 5.6.2 together with the observation that $Q^{\text{mid}}(\mathbf{k}, \mathbf{c}^\sharp) \in 0$, to find the following estimations for the remainders:

Corollary 5.6.3 *Let $f \in C^{1,1}(Cd)$ with $L(\text{rf})$ -Lipschitz gradient. Then, for the cubature formulas (5.13), (5.25), and (5.28), the following error estimates hold:*

$$E^{\text{mid}}(f) = \frac{Q_{\text{tr k. j}} c^2 k^2}{i 6 c L(rf)} \quad (5.63)$$

$$E_{\text{tr}}(f) = \frac{Q_{\text{tr}} k_{\text{ic}}^2}{1 - \frac{3}{6} \frac{1}{2} \textcircled{R} Q_{\text{tr}}^L(rf)} \cdot c^2 \quad (5.64)$$

$$\| \tilde{A} \|_{L(rf), 2} [0, 1/2] \leq C_2 \| A \|_{L(rf), 2} [0, 1/2]. \quad (5.65)$$

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

Corollary 5.6.3 indicates which one of the three cubature formulas (5.13), (5.25), and (5.28) has the smaller constant in its error estimate. We see that the best constant (minimal possible) in the error bound (5.65) is obtained by taking $\alpha = \frac{1}{2}$. This extremal value of the parameter

α provides the following cubature formula, which satisfies the upper Hermite–Hadamard inequality:

$$\frac{1}{j} \int_{C_d} f(\mathbf{x}) d\mathbf{x} \cdot Q^{\text{Ham}}(f) : \alpha = \frac{1}{2} Q^{\text{mid}}(f) \wedge \frac{1}{2} Q^{\text{tr}}(f). \quad (5.66)$$

In the one-dimensional case (5.66) reduces to

$$\frac{1}{b-a} \int_a^b f(t) dt \cdot \frac{1}{2} (f(a) + f(b)) : \alpha = \frac{1}{2} \left(\frac{f(a) + f(b)}{2} \right), \quad (5.67)$$

which was discovered by Hammer [14], but sometimes it is also attributed to Bullen [5], see [11, p. 11]. When C_d is the interval $[a, b]$ (and k, k is the absolute value), a short calculation reveals that from (5.63) and (5.64) we easily get, as mentioned in the Introduction, the corresponding classical bounds (5.2) and (5.4). Finally, we should mention, as in the univariate case, that the constant of the error in the trapezoidal cubature formula is twice as large as that for the midpoint cubature formula. Also, we immediately see that the constant in the latter is twice as large as for the new multivariate version (5.66) of Hammer's quadrature formula.

5.7 Numerical tests

In this section we provide some numerical tests, which we perform in order to validate our theoretical predictions and to compare the set of cubature formulas described in the previous sections. We also give another comparison with uniform and non-uniform centroidal Voronoi cubatures provided in the paper [4]. We should mention that these latter are cubature formulas of the standard form, which use a set of numerical values of the integrand at the center of gravity of each element in a subdivision. We shall abbreviate these cubature formulas as UCVC and CVC, respectively. Cubature formulas of this type have many useful general properties, see [4]. We have considered the following two bivariate test functions

$$f_1(x, y) = \frac{(x^2 + y^2)^2}{p},$$

$$f_2(x, y) = x + y + 1.$$

Within each cubature formula a different behaviour is observed, depending on the characteristics of the integrand. Note that f_1 is componentwise convex but f_2 is componentwise concave. Then from Corollary 5.4.3, we know that the midpoint and Hammer's cubature formulas are superior to the trapezoidal cubature formula for f_1 and f_2 . As we will see in the following, these theoretical predictions are confirmed by all our numerical tests.

In these experiments the integration domain is the unit square $[0, 1]^2$, which we divide into

N^2 equal subsquares. Then we apply a cubature formula to each subsquare. In the following tables, we present the behavior of error corresponding to each cubature formula with respect to the number of subdivisions in each direction N . In Table 5.1 we have displayed the cubature errors of the first test function above, (the corresponding number of subdivisions in each direction N appears in the first column). For completeness sake here are the errors for some larger value of N . In the remaining part of the chapter, The absolute value of the errors of the trapezoidal, midpoint, Simpson's, Hammer's, uniform and non-uniform centroidal Voronoi cubatures will be denoted respectively by

$$E_N^{\text{tr}}, E_N^{\text{mid}}, E_N^{\text{Sim}}, E_N^{\text{Ham}}, E_N^{\text{UCVC}}, E_N^{\text{CVC}}.$$

All results in the tables given below were generated by using Matlab software. The two examples of a mesh for the uniform and non-uniform centroidal Voronoi cubature formula were generated by using the Matlab routine "PolyMesher.m", included in [10].

N	E_N^{tr}	E_N^{mid}	E_N^{Sim}	E_N^{Ham}	E_N^{UCVC}	E_N^{CVC}
10	0.0044411	0.0022193	8.3333333e-07	0.0011109	0.0044372	0.0044
20	0.0011109	5.5537326e-04	5.2083333e-08	2.7776475e-04	0.0011107	0.0011
40	2.7776475e-04	1.3887750e-04	3.2552090e-09	6.9443631e-05	2.7774955e-04	2.7317e-04
80	6.9443631e-05	3.4721510e-05	2.0344926e-10	1.7361061e-05	6.9442678e-05	6.8201e-05
160	1.7361061e-05	8.6805112e-06	1.2714940e-11	4.3402747e-06	1.7361001e-05	1.7027e-05
320	4.3402747e-06	2.1701362e-06	8.0313534e-13	1.0850692e-06	4.3402711e-06	4.2485349e-06

Table 5.1 – The behavior of the error corresponding to each cubature formula for the test function f_1 .

Remark 5.7.1 As this table shows that this is close to theoretical predictions. It is clear from this example that the error of the centroidal Voronoi cubature formula is approximately the same as the trapezoidal cubature formula, which is approximately twice as large as the error of the midpoint cubature formula. This latter is also approximately twice as large as the error of the Hammer's cubature formula. Table 5.1 obviously shows that Simpson's cubature formula is very much better than all other cubature formulas. Finally, it is seen that whereas the Hammer's, Simpson's and the midpoint cubature formulas provide good errors, the centroidal Voronoi and the trapezoidal cubature formulas are far less accurate for small values of N . This shows that the choice of cubature formulas can result in orders of magnitude saving in computational time.

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

In the following graphs. We first draw the mesh corresponding to the centroidal Voronoi cubature formula for the uniform and non-uniform cases. We then draw the behavior's error of each cubature formula with respect to the number of subdivisions in each direction (in the left side), and also the log scale graph for every case (in the right side). The last graph gathers the behavior of all cubature formulas in order to facilitate the comparison.

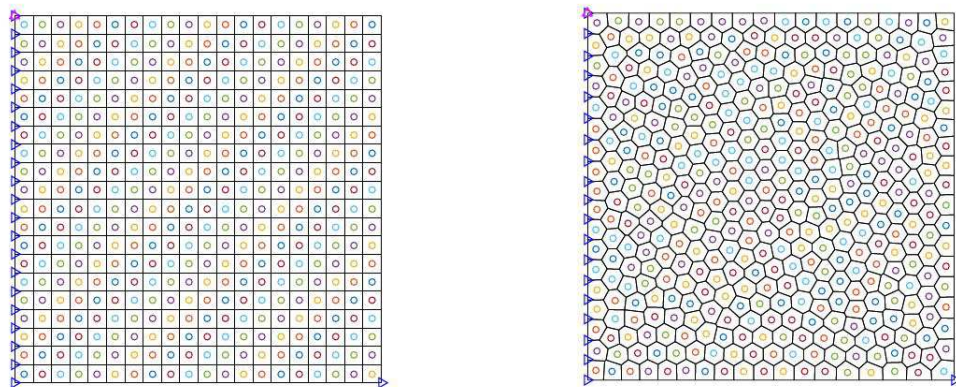


Figure 5.1 – Mesh of the unit square corresponding to the uniform centroidal Voronoi cu-bature formula (left), and that corresponding to the non-uniform centroidal Voronoi cu-bature formula (right). $N \in [20, 400]$ in these examples.

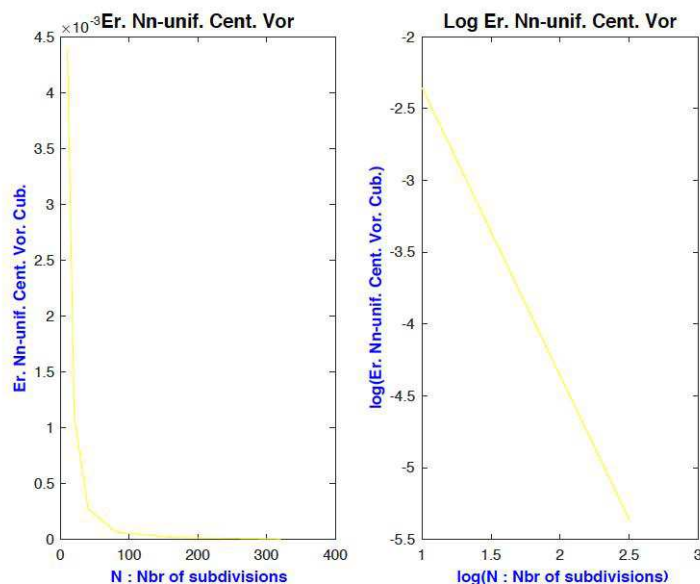


Figure 5.2 – Graph of the error corresponding to the approximation with the non-uniform centroidal Voronoi formula (left), and the error in the log scale (right).

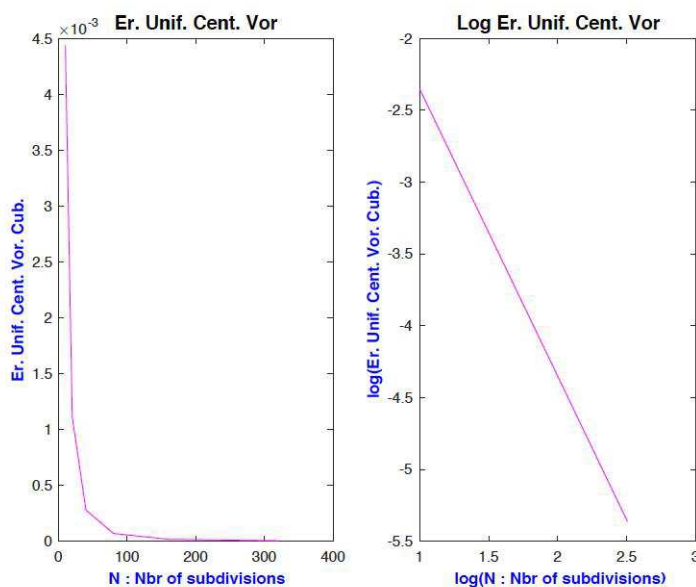


Figure 5.3 – Graph of the error corresponding to the approximation with the uniform cen-troidal Voronoi formula (left), and the error in the log scale (right).

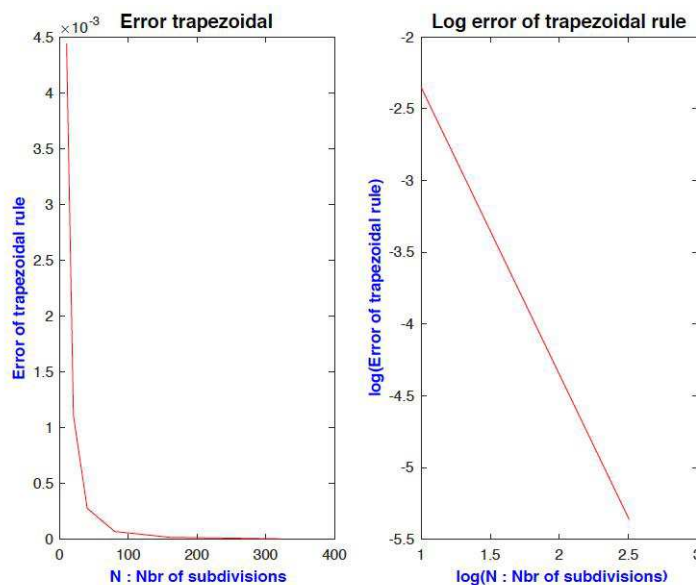


Figure 5.4 – Graph of the error corresponding to the approximation with the Trapezoidal formula (left), and the error in the log scale (right).

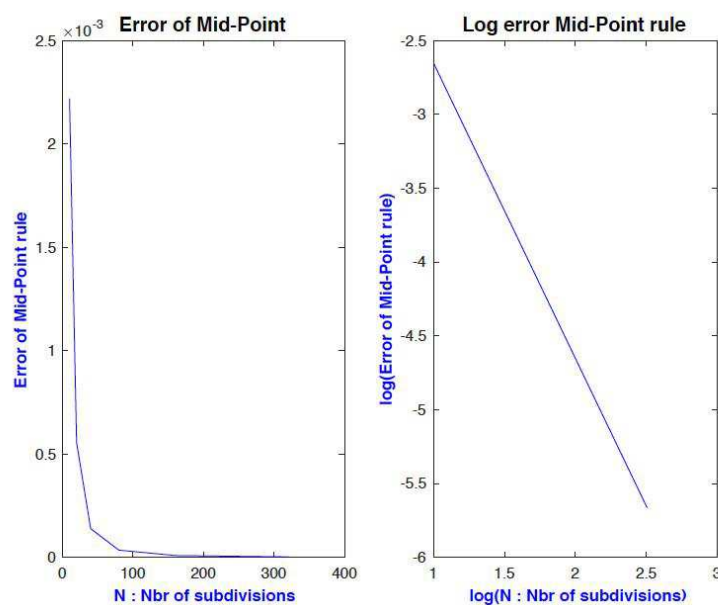


Figure 5.5 – Graph of the error corresponding to the approximation with the Midpoint for-mula (left), and the error in the log scale (right).

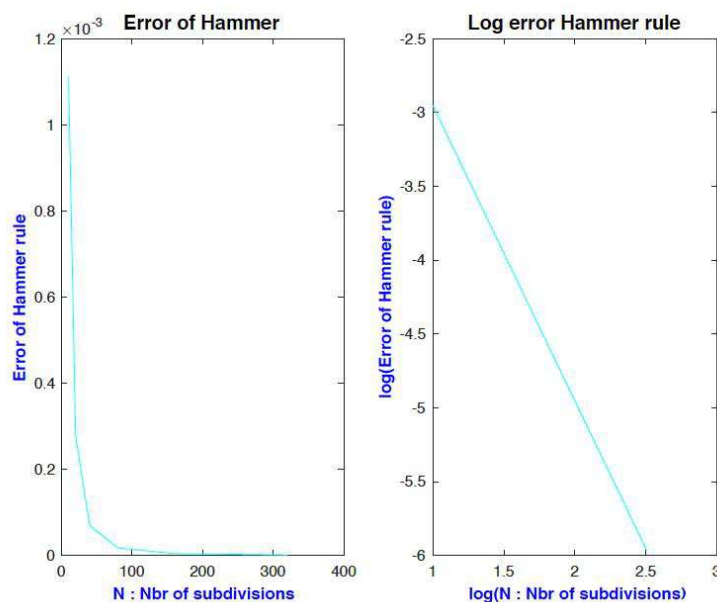


Figure 5.6 – Graph of the error corresponding to the approximation with the Hammer for-mula (left), and the error in the log scale (right).

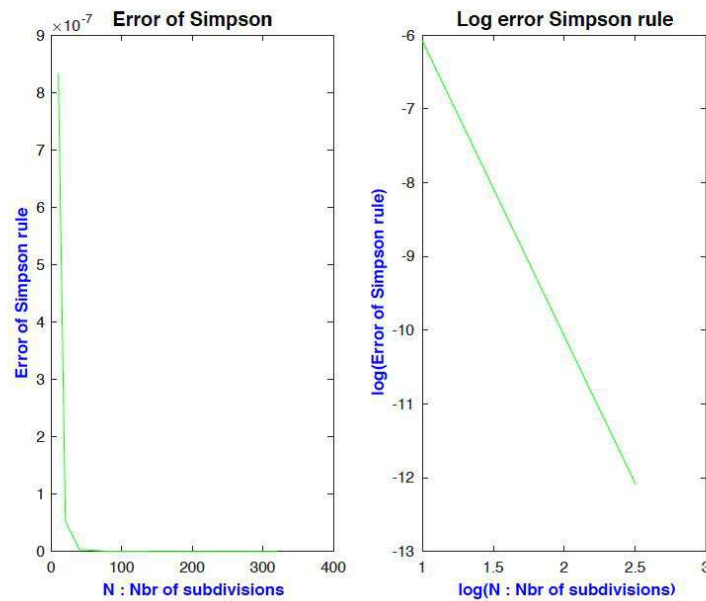


Figure 5.7 – Graph of the error corresponding to the approximation with the Simpson formula (left), and the error in the log scale (right).

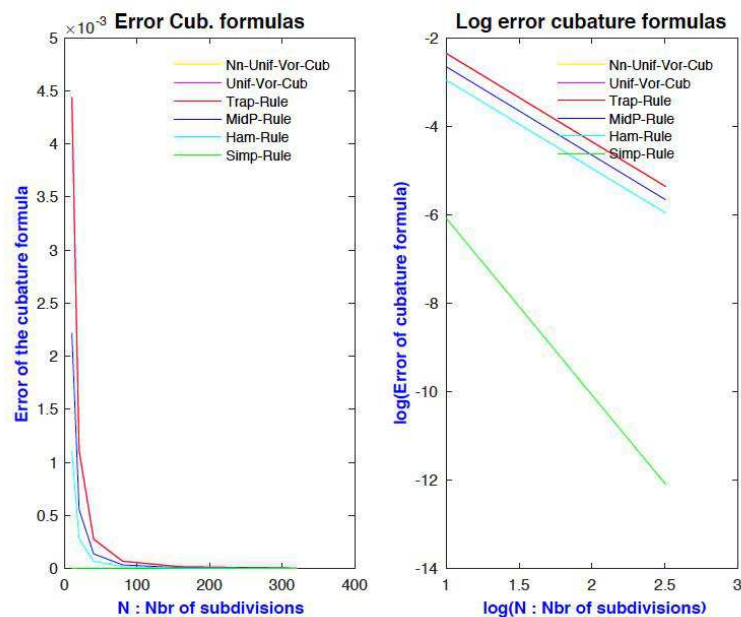


Figure 5.8 – Graph of the error corresponding to the approximation of each formula (left), and the error in the log scale (right).

The last graph confirms that Simpson's cubature formula is significantly superior to the all other cubature formulas (see Remark 5.7.1). However, we note that the graph corresponding to the centroidal Voronoi cubature formula is superimposed with that of trapezoidal cubature

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

formula. We remark also that the graph's error of Simpson's cubature formula is superimposed with the x-axis in the left figure since this latter generates a much smaller error in comparison with the error of the other cubature formulas.

Now, we present the second numerical test which will be carried out for the second function f_2 .

N	E_{tr} N	E_{mid} N	E_{Sim} N	E_{Ham} N	E_{UCVC} N	E_{CVC} N
10	8.0296770e-05	4.0142077e-05	4.2049058e-09	2.0077347e-05	8.0263169e-05	7.6748e-05
20	2.0077347e-05	1.0038279e-05	2.6318858e-10	5.0195340e-06	2.0075242e-05	1.9698e-05
40	5.0195340e-06	2.5097424e-06	1.6452173e-11	1.2548959e-06	5.0194026e-06	4.9193e-06
80	1.2548958e-06	6.2744641e-07	1.0100809e-12	3.1372471e-07	1.2548876e-06	1.2245e-06
160	3.1372474e-07	1.5686227e-07	7.3496764e-14	7.8431242e-08	3.1372423e-07	3.0668e-07
320	7.8431285e-08	3.9215699e-08	3.9523940e-14	1.9607791e-08	7.8431341e-08	7.6624957e-08

Table 5.2 – The behavior of the error corresponding to each cubature formula for the test function f_2 .

In contrast to the previous example, here already for small values of N all cubature formulas give significantly smaller errors. However, we see that the superiority of Simpson's cubature formula over all other cubature formulas is still obvious. Note again that the trapezoidal cubature formula tends to be slightly closer to than the centroidal Voronoi cubature formula, but neither is as close with $N \approx 320$ as Simpson's cubature formula is with $N \approx 10$.

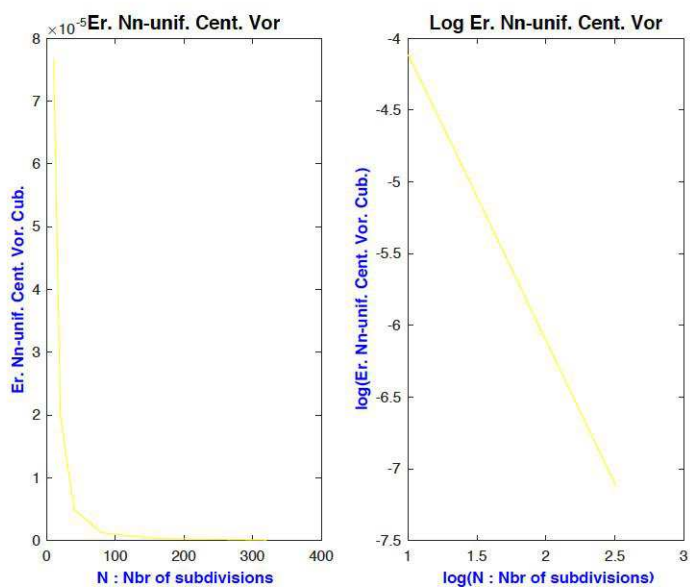


Figure 5.9 – Graph of the error corresponding to the approximation with the non-uniform centroidal Voronoi formula (left), and the error in the log scale (right).

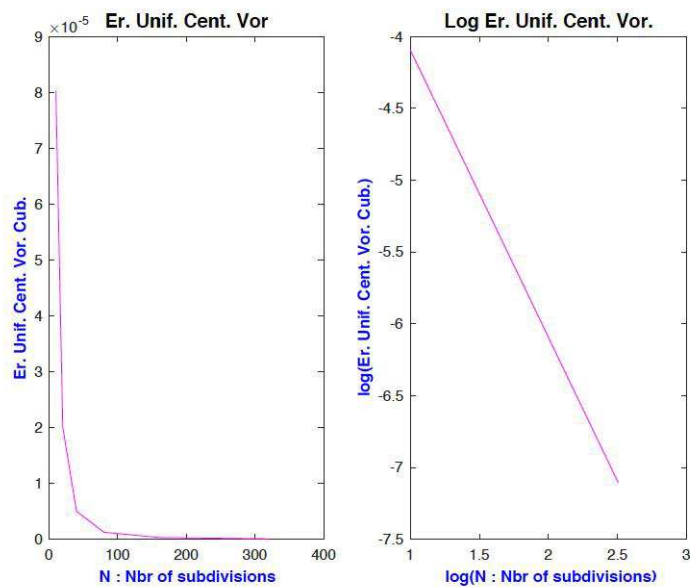


Figure 5.10 – Graph of the error corresponding to the approximation with the uniform centroidal Voronoi formula (left), and the error in the log scale (right).

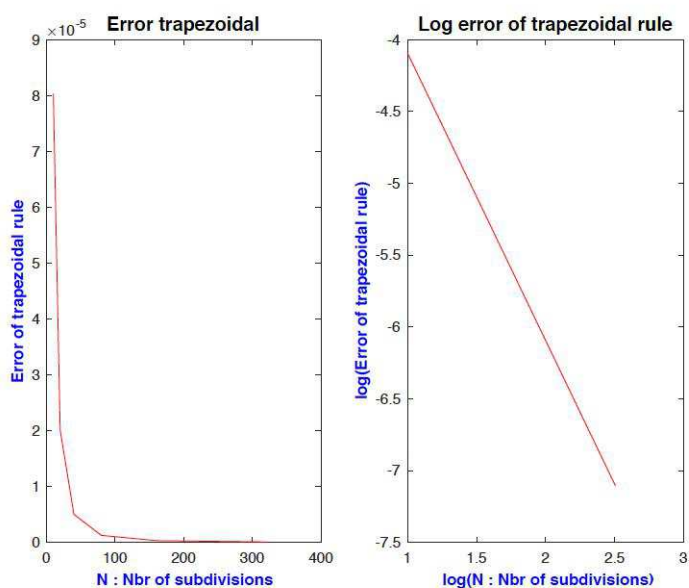


Figure 5.11 – Graph of the error corresponding to the approximation with the Trapezoidal formula (left), and the error in the log scale (right).

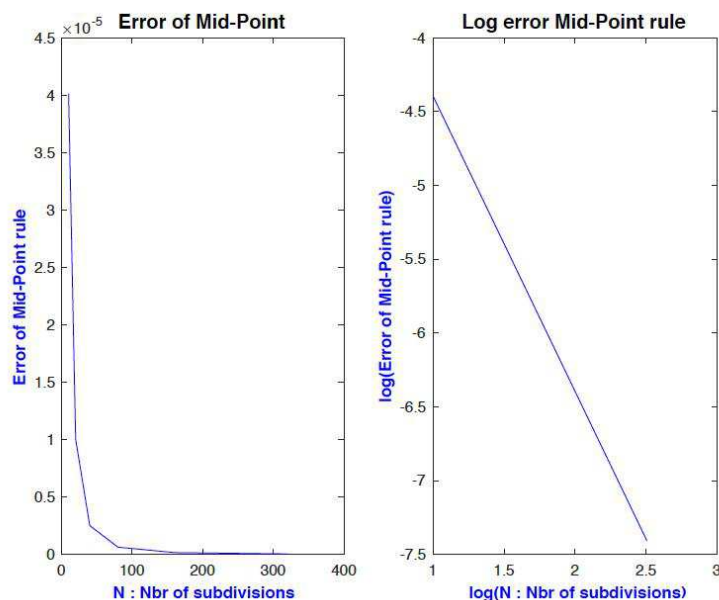


Figure 5.12 – Graph of the error corresponding to the approximation with the Midpoint formula (left), and the error in the log scale (right).

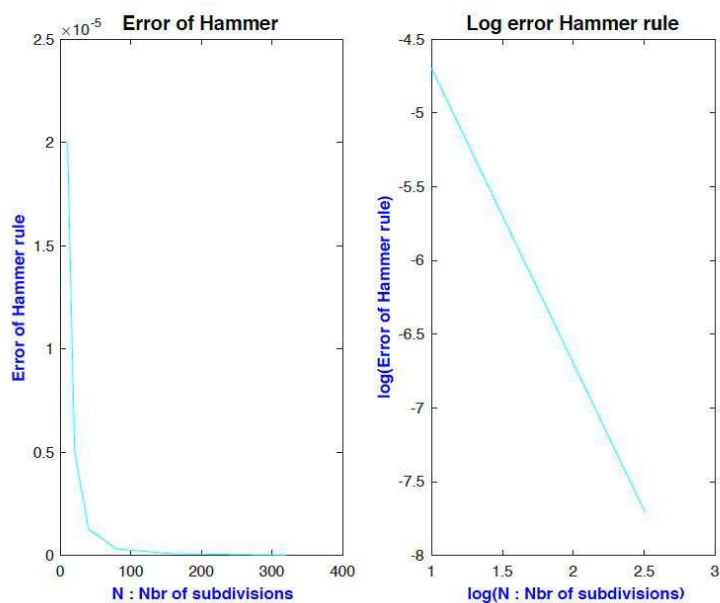


Figure 5.13 – Graph of the error corresponding to the approximation with the Hammer formula (left), and the error in the log scale (right).

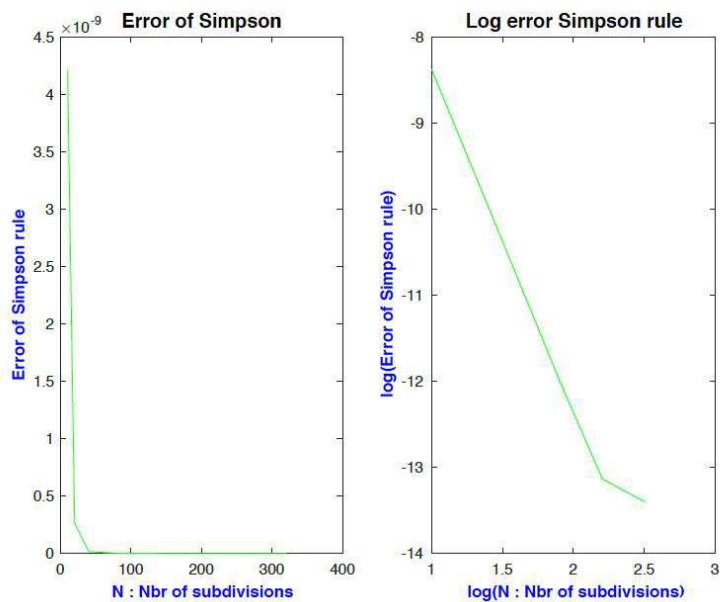


Figure 5.14 – Graph of the error corresponding to the approximation with the Simpson formula (left), and the error in the log scale (right).

New Cubature formulas and Hermite-Hadamard type inequalities using integrals over some hyperplanes in the d -dimensional hyper-rectangle

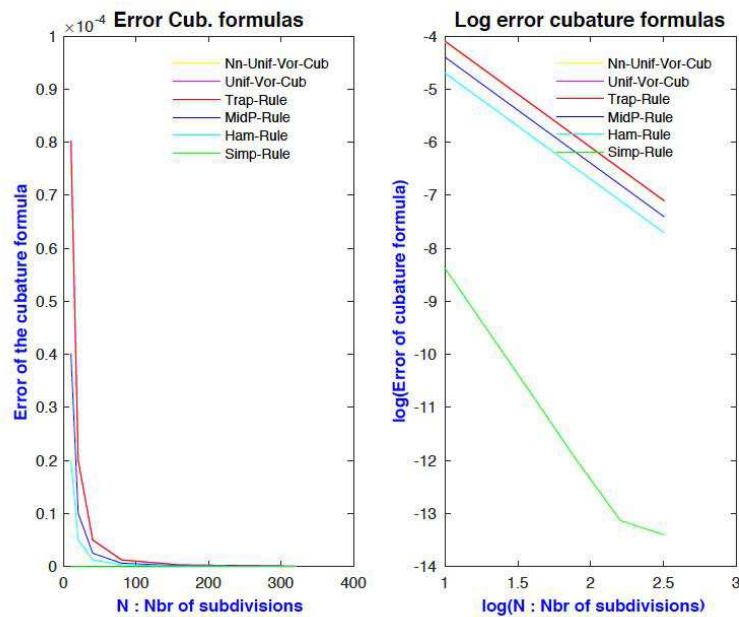


Figure 5.15 – Graph of the error corresponding to the approximation of each formula (left), and the error in the log scale (right).

We can deduce also from the graphs of this second numerical test the same interpretation as the first test.



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Conclusions, final remarks, implications and extensions

Because of the fact that our main results appeared in chapters three, four and five, therefore, we will talk about this chapters briefly and separately to mention the main results and final remarks of each chapter. Conclusions were arranged as follows:

In chapter three, we are present a new and efficient way of approximating a given function of multiple variables by linear operators, which approximate all *strongly* convex functions from above (or from below). This additional information is used to characterize sharp error estimates for continuously differentiable functions with Lipschitz continuous gradients. All the proposed error estimates are controlled by the Lipschitz constants of the gradients and the error associated with using the quadratic function. Moreover, if the function to be approximated is also strongly convex then we establish sharp upper as well as lower refined bounds for the error estimates. Also, the numerical experiments in this chapter clearly demonstrate that the strong convexity of strongly convex function has been preserved and there is no visual difference between the test function and its piecewise-linear interpolant, as we have seen in **Figs 3.1, 3.2 and 3.3**. **Furthermore**, we have noticed the accuracy of our implementation of barycentric approximation, as we stated in section 3.5 (see the Tables 3.1, 3.2, 3.3 and 3.4), where we have seen that, for all test functions, the MSE decreases with increasing numbers of nodes as N increases. Actually, the motivation that caused our attention to such class of functions is that these functions are used widely in economic theory (see [1]), and are also central to optimization theory (see [2]). Indeed, in the framework of function minimization, this convexity notion has important and well-known implications.

In chapter four, we are present a new classes of cubature formulas (which we call them strongly positive, respectively negative, definite cubature formulas) for numerical integration (or multidimensional quadrature), that approximate from above (or from below) the exact value of the integrals of every function of multiple variables having a certain type of convexity. In fact, we got two characterization results of any linear functional $C^{1,1}(-) : \mathbf{R}$, which is nonnegative on the set of convex functions, then we apply this results to the case when the functional is the error functional of our cubature formulas. We concluded that, for functions

belonging to $C^{1,1}(\cdot)$, the error estimates based on such cubature formulas may always be controlled by the Lipschitz constants of the gradients, the different types of convexity and the error associated with using the quadratic function. In addition, when we know that the function to be integrated satisfies the classical convexity or strong convexity, we use this additional information to establish sharp upper as well as lower refined bounds for the error estimates for these classes of functions. With regard to the strongly positive definite cubature formulas, we give characterization results between them and the partition of unity of the integration domain, also explain how we can construct them using decomposition method for domain integration. The same thing is achieved for strongly negative definite cubature formulas, where we characterize them in two different ways: the first one by certain partitions of unity and the second one by a class of positive linear operators. We also present practical construction of strongly negative definite cubature formulas. Further, we show that there is a main difference between them and strongly positive definite cubature formulas. Indeed, we noted that the latter (strongly negative definite cubature formulas) can exist only if the domain of integration is a convex polytope. By means of the numerical examples which are provided in this chapter, we illustrated the efficiency of our cubature formulas. For more details we can see the tables and figures in section 4.4 which explain that clearly.

In chapter five, according to the results given in the tables, Simpson's cubature formula, i.e., average cubature formula with $\mathcal{A} \in \mathcal{E}_3^2$ derived in this chapter, provides more accurate results, than the other average cubature formulas. This behavior has also been observed for numerous other integrands. This is not surprising, since Simpson's cubature formula is of order 3 while the other average cubature formulas are of order 1. In comparing the numerical results, we have also observed that the non-uniform centroidal Voronoi cubatures of the standard form, which use the values of the integrand at certain points, give the worst results. Note however that the use of the non-uniform centroidal Voronoi cubature produces slightly better results than the uniform one.

The cubature formulas we have presented have applications to the theory and practice of the numerical solution of PDEs using the so-called non-conforming Crouzeix–Raviart element. In a forthcoming paper, see [1], we have used cubature formulas of this type for the approximate solution of a planar elasticity problem. In fact, that there are many other applications, especially in experimental physics and engineering, where the standard discrete sample values from functions are not available, but only their mean values are accessible. For instance, this data type appears naturally in computer tomography with its many applications in medicine, radiology, geology, amongst others.

We now allude briefly to further extensions which are possible. Throughout the work we have considered, cubature formulas, which use a number of integrals over certain hyperplane sections parallel to coordinate hyperplanes. We shall describe the general problem elsewhere when certain prescribed hyperplane sections are not necessary parallel to coordinate hyperplanes. Let us note that our Theorem 5.6.2 provides in this general context sharp error bounds with explicit constants.

Conclusions, remarques finales, implications et extensions

Dans la présente thèse, nous avons étudié plusieurs questions liées à l'approximation des fonctions de plusieurs variables par de nouveaux types d'opérateurs linéaires, qui gardent un signe constant pour toute fonction satisfaisant une certaine convexité généralisée. Les principaux résultats de ce travail apparaissent dans les chapitres trois, quatre et cinq. Dans ce chapitre nous allons faire une synthèse des chapitres précédents en présentant brièvement les principaux résultats et remarques finales de chaque chapitre. Les conclusions ont été disposées comme suit:

Dans le chapitre trois, nous avons présenté des opérateurs linéaires, qui gardent un signe constant pour toutes les fonctions fortement convexes. Cette information supplémentaire a été utilisée pour caractériser la meilleure estimation de l'erreur pour les fonctions continues différentiables ayant des gradients Lipschitz continus. Toutes les estimations d'erreur proposées sont contrôlées par les constantes de Lipschitz des gradients et l'erreur associée à l'utilisation de la fonction quadratique. De plus, si la fonction à approcher est également fortement convexe, nous avons établi des bornes supérieures et inférieures explicites pour les estimations d'erreur. Les expériences numériques présentées dans le chapitre montrent clairement que la convexité forte des fonctions tests a été préservée et qu'il n'y a pas de différence visuelle entre ces dernières et ses interpolants linéaires par morceaux. Nous nous référons aux figures 3.1, 3.2 et 3.3. De plus, nous avons remarqué la bonne qualité de l'approximation barycentrique, comme nous l'avons indiqué à la section 3.5 (voir les tableaux 3.1, 3.2, 3.3 et 3.4). En fait, le point qui a attiré notre attention sur une telle classe de fonctions est que ces fonctions sont largement utilisées dans la théorie des mathématiques pour la compréhension des phénomènes économiques (voir [1]), et sont également essentielles à la théorie de l'optimisation (voir [2]). En effet, dans le cadre de la minimisation des fonctions, cette notion de convexité a des implications importantes et bien connues.

Dans le chapitre quatre, nous avons présenté une nouvelle classe de formules de quadrature multidimensionnelle (que nous avons appelées formules de quadrature fortement définies positives (respectivement définies négatives), qui conduisent à des valeurs approchées par

excès (respectivement par défaut) de l'intégrale des fonctions ayant un certain type de convexité. Ainsi, nous avons obtenu deux résultats de caractérisation de toute fonctionnelle linéaire $C^{1,1}(\cdot) \rightarrow \mathbf{R}$, qui est positive sur l'ensemble des fonctions convexes. Nous avons appliqué ces résultats au cas où la fonctionnelle associée à de nos formules de quadrature. Nous avons montré que, pour les fonctions appartenant à $C^{1,1}(\cdot)$, les estimations d'erreur basées sur ces formules de quadrature peuvent toujours être contrôlées par les constantes de Lipschitz des gradients, les différents types de convexité et l'erreur associée à l'utilisation de la fonction quadratique. De plus, la fonction à intégrer satisfait la convexité classique ou la convexité forte, ceci nous permet d'établir des bornes supérieures et inférieures explicites pour les estimations d'erreur pour ces classes de fonctions. En ce qui concerne les formules de quadrature définies fortement positives, nous avons donné des résultats de caractérisation avec la partition de l'unité du domaine d'intégration. Nous avons aussi expliqué comment nous pouvons les construire en utilisant la méthode de décomposition pour l'intégration de domaine. Nous avons caractérisé les formules de quadrature définies fortement négatives de deux manières différentes: la première par certaines partitions d'unité et la seconde par une classe d'opérateurs linéaires positifs. Nous avons aussi proposé une méthode pour la construction pratique de ses formules de quadrature. En effet, nous avons noté que ces dernières (formules de quadrature définies fortement négatives) ne peuvent exister que si le domaine d'intégration est un polytope convexe. À l'aide des exemples numériques présentés dans ce chapitre, nous avons illustré l'efficacité de nos formules de quadrature. Pour plus de détails, on renvoie aux tableaux et figures de la section 4.4 qui montrent cela clairement.

Dans le chapitre 5, en se basant sur les résultats des tests numériques, la formule de quadrature multidimensionnelle de Simpson, c'est-à-dire la formule de quadrature associée comme en dimension 1 au paramètre $\otimes \mathcal{A}^2_3$ établie dans ce chapitre, produit des résultats plus précis que les autres formules de quadrature. Ce comportement a également été observé pour de nombreuses fonctions-test. Cela n'est pas surprenant, puisque la formule de quadrature de Simpson est d'ordre 3 alors que les autres formules cubiques sont d'ordre 1. En comparant les résultats numériques, nous avons également observé que les quadrature de type Voronoi centrées non uniformes donnent les résultats les moins satisfaisants. Notons cependant que l'utilisation de la quadrature non-uniforme de type Voronoi centrées produit des résultats légèrement meilleurs que celle basée sur une triangulation uniforme.

Les formules de quadrature que nous avons présentées ont des applications pour la résolution des équations aux dérivées partielles connues sous le nom de l'équation générale de comportement de l'élasticité linéaire. Ainsi c'est le cas des solutions numériques des EDP en utilisant l'élément fini de Crouzeix-Raviart non conforme, voir [1]. En fait, il existe de nombreuses autres applications, en particulier en physique expérimentale et en ingénierie, où les valeurs d'échantillons discrets standards de fonctions ne sont pas disponibles, mais seulement leurs valeurs moyennes sont accessibles. Par exemple, ce type de données apparaît naturellement dans la tomographie par ordinateur avec ses nombreuses applications en médecine, en radiologie, en géologie, entre autres.

Nous allons maintenant faire brièvement allusion à d'autres extensions possibles. Tout au long du travail que nous avons présentés, les formules de quadrature utilisent un certain nombre d'intégrales sur certaines sections hyperplanes d'un hyper-rectangle. Nous avons établi un résultat général de majoration d'erreur lorsque certaines sections d'hyperplanes prescrites ne sont pas nécessairement parallèles aux hyperplans de coordonnées. Notons que le théorème 5.6.2 fournit dans ce contexte général des bornes d'erreur avec des constantes explicites.

Enfin, les principales perspectives de recherche, à plus court terme, qui apparaissent à l'issue de cette thèse concernent l'extension de ces résultats à d'autre type de convexité généralisée, par exemple, la convexité uniforme. Nous envisageons par la suite d'étendre les formules de quadrature multidimensionnelle au cas où certaines intégrales sont connues sur chaque facette d'une triangulation simpliciale.

