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Computational Geometry of
Positive Definite Quadratic
Forms

Polyhedral Reduction Theories,
Algorithms, and Applications

Achill Schürmann



American Mathematical Society

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For Ida, Jannis and Kristina

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Preface

The *Geometry of Positive Definite Quadratic Forms* is a rich and old subject which arose in the arithmetic studies of quadratic forms. Through the seminal works of Minkowski and Voronoi a century ago, the geometric viewpoint became predominant. The study of arithmetical and inhomogeneous minima of positive definite quadratic forms turned into a study of lattice sphere packings and coverings. Lattices and, more generally, periodic (point) sets are by now widespread in mathematics and its applications. The important monograph “Sphere packings, Lattices and Groups” [69] by Conway and Sloane, with its over 100 pages of references, shows exemplarily the influence on other mathematical disciplines. This becomes particularly apparent for the 24-dimensional Leech lattice and its connections to number theory, group theory, coding theory and mathematical physics. Since the complexity of problems grows with the dimension, it is no surprise that over the past decades more and more computer support was used to study higher dimensional lattices and more general structures. Still, the *Geometry of Positive Definite Quadratic Forms* is an essential tool, not only in the study of lattice sphere packings and coverings.

One aim of this book is to give a nearly self-contained introduction to this beautiful subject. We present the known material with new proofs, which then admit natural generalizations. These extensions of the known theory were mainly targeted to support the study of extreme periodic sets. However, it turned out that the resulting new theory has other applications as well, as for example, the classification of totally real thin number fields. On the way, always an eye is kept on computability; algorithms are developed that allow computer assisted treatments. Using tools from combinatorial, from linear and from convex optimization, many difficult problems become accessible now. This is, for example, demonstrated in the search for new currently best-known lattice sphere coverings and in the classification of 8-dimensional perfect lattices, which previously was thought to be impossible with the known methods.

Although this book deals with classical topics which have been worked on extensively by numerous authors, it shows exemplarily how computers may help to gain new insights. On the one hand it is shown how computer assisted (sometimes heuristic) exploration helps to discover new exceptional structures. In many cases these would probably not have been found without a computer. On the other hand several computer assisted proofs are given, which deal with extraordinarily large data or involve large enumerations. It is shown how proofs can be obtained from numerical results, by postprocessing of roundoff solutions. All of these aspects of computer mathematics are nowadays supported by a growing functionality of computer algebra systems and by an increasing number of reliable small programs for specific purposes. In some cases one has to combine, to supplement and to improve on existing software tools. If solutions for basic tasks are obtained they should be

made accessible to the growing community of computer enthusiastic mathematicians. Underlying many of the presented computational results are in particular two such programs: A program for rigorous determinant maximization (including semidefinite programming) allowing exact certified error bounds, and secondly, a program for polyhedral representation conversion under symmetries.

Computer assisted mathematical explorations and proofs are of increasing importance in many areas of modern mathematics. Even close to the topics of this book there have been amazing developments recently. An example is the proof by Hales [129], [130] of the famous Kepler conjecture. Several exciting results have been obtained in the context of *linear and semidefinite programming bounds* for spherical codes and point sets in Euclidean spaces. There is the new sphere packing bound by Cohn and Elkies [60], and based on it, the proof by Cohn and Kumar [63] (see also [61]) that the Leech lattice gives the best lattice sphere packing in 24 dimensions. There is the proof of Musin [185] showing that the kissing number in four dimensions is 24 (see [197] for an excellent survey). Shortly after, Bachoc and Vallentin [6], gave more general, new bounds on the size of spherical codes. Their works are followed by similar approaches for other problems, using semidefinite programming. As in some parts of this book, these works involve numerical computations which are then turned into mathematical rigorous proofs. Often numerical quests and subsequent mathematical analysis lead to new mathematical insights. A fascinating example is the study of *universally optimal point configurations*, recently invoked by Cohn and Kumar [62] (see also [9] and [264]). Although all of this is happening literally next door to the topics of this book, I decided to keep it focused as it is. Adequate treatments will hopefully fill other books in the near future. For now I encourage the reader to study the great original works.

Acknowledgments. This book grew out of lectures held at an Oberwolfach Seminar on Sphere Packings and at the University of Magdeburg, together with parts of research articles which were previously published, in a similar or partially different form (see [45], [95], [225], [226], [228], [229]). I thank my coauthors David Bremner, Francisco Santos Leal and in particular Mathieu Dutour Sikirić and Frank Vallentin for their many contributions and their shared enthusiasm for the subject. I thank Frank, Mathieu, Henry Cohn, Slava Grishukhin, Jeff Lagarias and Jacques Martinet for their very helpful feedback on prior versions.

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Overview

This overview is intended to guide through the topics and results of this book. Definitions and explanations for used terminology can be found with help of the index. Readers not so familiar with the treated topics may perhaps start by looking into the introductory material in Chapter 1 and Sections 2.1, 3.1 and 4.1. Most of the results in this book are described in the language of positive definite quadratic forms because it is the basis for most computations. In the following summary we nevertheless primarily use “lattice-terminology”, since it is more common nowadays. References to the literature can be found in the corresponding context of the book.

Chapters 1 and 2: An introduction. The first two chapters are mainly introductory and contain, in contrast to the remaining chapters, only a few new results.

In the first chapter we briefly recall the history of the theory of positive definite quadratic forms and its natural connection to the lattice sphere packing problem. Along the way, we introduce to basic notions and results used in the following chapters. In Sections 1.2, 1.3 and 1.4 we review known results of our main aimed at applications: the sphere packing, the sphere covering and the (simultaneous) sphere packing-covering problem. For all three problems there is a notorious open question: *Do there exist dimensions in which lattices do not give optimal configurations?* This problem is one of our main motivations to extend Voronoi’s (lattice) reduction theories in Chapter 3 and Chapter 4.

The second chapter deals with several aspects of Minkowski’s reduction theory, which in a sense is a prototype for other polyhedral reduction theories. In Section 2.1, we start with a short discussion about reduction in general, and then introduce Minkowski’s theory in Section 2.2. We in particular give a previously unknown, non-redundant description of Minkowski’s polyhedral reduction domain up to dimension 7. In Section 2.3 we describe relations to Minkowski’s successive minima and state a challenging conjecture concerning an improvement of a classical and central theorem in the Geometry of Numbers. In Section 2.4 we end the second chapter with an application of Minkowski reduction to multidimensional continued fraction expansions, used for simultaneous Diophantine approximations.

Chapter 3: Voronoi’s first reduction theory. In Section 3.1 we start by introducing to the theory of perfect lattices, respectively to “Voronoi’s first reduction theory”. Based on so-called *Ryshkov polyhedra*, we give complete proofs for the theory and explain Voronoi’s algorithm. We provide some background on computational tools (such as the shortest vector problem and isometry tests for lattices), which were recently used to finish the classification of perfect lattices up to dimension 8.

Our treatment of Voronoi’s theory is presented in a way such that it can be generalized naturally from a lattice theory to a theory for m -periodic point sets. As lattices can be viewed as linear images of \mathbb{Z}^d in \mathbb{R}^d , m -periodic sets are linear images of a *standard periodic set*

$$(0.1) \quad \bigcup_{i=1}^m \mathbf{t}_i + \mathbb{Z}^d \quad \text{with} \quad \mathbf{t}_i \in \mathbb{R}^d.$$

In Section 3.2, we introduce a new parameter space $\mathcal{S}_{>0}^{d,m}$ to deal with m -periodic sets in \mathbb{R}^d up to isometries. We introduce *generalized Ryshkov sets*, on which determinant minimization yields the densest m -periodic sphere packings.

In Section 3.3 we analyze local optima (m -extreme periodic sets) of the packing density in $\mathcal{S}_{>0}^{d,m}$. We obtain necessary and sufficient conditions. It turns out that our framework provides a new explanation for a previously by Conway and Sloane observed phenomenon; namely for the existence of uncountably many 9-dimensional 2-periodic sphere packings (fluid diamond packings) which are as dense as the densest known lattice sphere packing. We investigate the possibility of improving the densest lattices (represented as points in $\mathcal{S}_{>0}^{d,m}$) locally, to obtain a periodic non-lattice set with larger packing density. We show that this is not possible (see Corollary 3.18). More generally, we show in Theorem 3.17 that a perfect, strongly eutactic lattice is *periodic extreme*, that is, it cannot locally be improved to a denser periodic point set.

In Section 3.4 we give extensions of Voronoi’s algorithm, hereby laying the theoretical foundations for systematic, computer assisted searches for dense periodic sphere packings. We develop a “ \mathbf{t} -theory” which enables us to find local sphere packing optima (\mathbf{t} -extreme sets) among all \mathbf{t} -periodic point sets. These are linear images of a standard periodic set (0.1) with a fixed translational part $\mathbf{t} = (\mathbf{t}_1, \dots, \mathbf{t}_m)$. For the case of a rational matrix \mathbf{t} we show in Theorem 3.23, in analogy to the classical theory, that there exist only finitely many \mathbf{t} -extreme sets. These can be enumerated by a generalized Voronoi algorithm. On top of the \mathbf{t} -theory, we extend the theory of G -perfect and T -perfect lattices (where G is a finite subgroup of the orthogonal group and T is a linear subspace in the space of quadratic forms).

This allows us to restrict searches for dense \mathbf{t} -periodic sphere packings to ones with specific features, for example with a fixed finite symmetry group. For rational \mathbf{t} and a finite subgroup of the orthogonal group (leaving (0.1) invariant) we show in Theorem 3.25 that there exist only finitely many local optima among sphere packings with the corresponding properties. This generalizes works of Bergé, Martinet, Sigrist and others. Our proof relies on a general observation (Lemma 3.26) regarding group actions on polyhedral subdivisions. The section ends with three examples of the G -theory, describing new results for Eisenstein, Gaussian and Hurwitz quaternionic lattices.

Chapter 4: Voronoi’s second reduction theory. In the fourth chapter we generalize Voronoi’s second reduction theory which is based on Delone polyhedra and Delone subdivisions of lattices. In Section 4.1 we first give the necessary definitions, some background and we explain Voronoi’s theory on secondary cones (also called L -type domains). We give a simplified and generalized proof for Voronoi’s theory in Section 4.2. Theorem 4.7 extends Voronoi’s theory to a “ \mathbf{t} -theory” for Delone subdivisions having a standard periodic vertex-set (0.1). For rational \mathbf{t} we

show that there exist only finitely many non-equivalent secondary cones (see Theorem 4.13). This gives a foundation for systematic searches for thin periodic sphere coverings. Another application is a possible search for “good” periodic quantizers.

In Section 4.3 we introduce an “equivariant G -theory” for secondary cones and, more general, a theory of T -secondary cones, in analogy to the theory of G -perfect and T -perfect periodic sets described in Section 3.4. As in Section 3.4 we derive from Lemma 3.26 a finiteness result for rational t and finite symmetry groups G (see Theorem 4.19). We put special efforts into an explicit description on how to obtain all Delone subdivisions of lattices and periodic sets within the G - and T -theory (see in particular Theorem 4.15 and the algorithms in Section 4.3.4). This practicability of our results is of great importance for the applications in Chapter 5.

In Section 4.4 we introduce the secondary cones of single Delone polyhedra and polyhedral complexes. We propose an algorithm to decide whether or not a given simplex with integral vertices is Delone for some positive definite quadratic form. It can possibly serve as a tool to classify lattice Delone simplices (up to $\text{GL}_d(\mathbb{Z})$ -equivalence) of a given dimension. We show that the number of inequivalent Delone simplices increases dramatically with the dimension, by constructing Delone simplices with relative volume increasing super-exponentially with the dimension. Previously only linear growth was known.

Chapter 5: Local analysis of coverings and applications. In the fifth chapter we harvest the fruits of Chapter 4 and apply them to obtain several results in context of the lattice sphere covering problem. The first two sections have a preparatory character.

In Section 5.1 we formulate algorithms that allow to solve (in principle) the lattice sphere covering and packing-covering problem in a given dimension by solving a finite number of convex optimization problems. We give explicit descriptions of determinant maximization and semidefinite programs. They are subject to linear matrix inequalities expressing that the covering radius of an underlying periodic set is bounded by some given constant (see Proposition 5.5). We describe the software tools we developed to find local lattice covering and packing-covering optima (or at least for generating certified bounds on their covering density or packing-covering constant).

In Section 5.2 we provide tools for a detailed local analysis. These allow to check for local optimality of a lattice, if necessary computationally. Using convex optimization software, we sometimes only have certified ranges for the actual locally optimal value. We show how this restricted information can nevertheless be used to obtain structural informations about the actual local optimizers. We derive quickly computable, local lower bounds for the lattice covering density and the packing-covering constant, applicable to all lattices having a given collection of Delone simplices. For some lattices (as seen for the Leech lattice in Section 5.5) these bounds can be tight (for the right choice of simplices attaining the covering radius). Hence they have the potential to prove local optimality of a lattice.

In Section 5.3 we explain how the tools from the previous two sections can be used to find new best known lattice coverings and packing-coverings. Our techniques enable us in particular to confirm all previously known results up to dimension 5. It is notable that these were previously obtained (without computer assistance) in many years of work and on hundreds of published pages. Beyond the previously known, we extend the knowledge up to dimension 5 by additional information

on all local optima. Although the lattice covering and the lattice packing-covering problem have both not been solved in dimension 6 so far, we describe conjecturally optimal lattices obtained by heuristic methods (see Section 5.3.3). Both lattices have the property that their Delone triangulation refines the Delone subdivision of the lattice E_6^* . As a first step in direction of a proof for global optimality, we prove computationally by a branch-and-bound method that the conjectural optimal covering lattice is the unique optimum among lattices having this refinement property (see Theorem 5.28). In many cases it is a problem to obtain exact coordinates for the new lattices. Exemplarily we show how to obtain exact coordinates for the new conjectural optimal 6-dimensional packing-covering lattice. We describe a new conjecturally optimal 7-dimensional covering lattice whose corresponding positive definite quadratic forms are (to our surprise) even rational (see Section 5.3.5). We describe how we obtained new, currently best known covering lattices in dimensions $d \geq 9$. These computations are based on our new T -secondary cone theory.

In Section 5.4 we apply the theory of T -secondary cones to a problem in algebraic number theory: the classification of all totally real thin algebraic number fields. Our classification is based on a list of 17 candidates, previously given by Bayer-Fluckiger and Nebe. By proving lower bounds on the covering density of positive definite quadratic forms in an associated linear subspaces T we exclude three of the candidates. This finishes the classification.

In Section 5.5 we take a closer look at two of the most exceptional lattices (in low dimensions): The root lattice E_8 and the Leech lattice. We show that both lattices are rigid, meaning they are uniquely determined by the type of their Delone subdivision. By applying our local lower bounds we show that the Leech lattice is a local lattice covering and packing-covering optimum. This shows in particular the existence of rigid, locally optimal lattice coverings, which affirmatively answers a long standing open question of Dickson (1968). The same method can not be applied to the E_8 root lattice. In fact, a local analysis reveals that it is not even a locally optimal covering lattice. In connection with a proof of this fact, we find a new currently best known 8-dimensional covering lattice (see Section 5.5.6).

In Section 5.6 we continue the investigation of lattices similar to E_8 , revealing a previously unknown phenomenon: The existence of local lattice covering maxima, for which we derive necessary and sufficient conditions. Based on them we prove computationally that the E_6 root lattice is the only lattice covering maximum in dimensions less or equal to 6, aside of \mathbb{Z} (which trivially is at the same time a 1-dimensional lattice covering optimum). The E_8 root lattice itself turns out to be only “almost” a local lattice covering maximum: Almost any, but not every local change of an associated positive definite quadratic form yields a lower covering density. We baptize these lattices *covering pessima* and prove that a lattice is a covering pessimum, if the Delone polytopes attaining its covering radius are all regular cross polytopes. This is for example the case for the root lattices D_4 and E_8 .

In Section 5.7 we consider local lattice covering maxima within a linear subspace T in the space of (associated) quadratic forms. We show a connection to the famous *Minkowski conjecture*, respectively to the so-called *covering conjecture*. Based on our new T -secondary cone theory we obtain an algorithm which can be used to verify or falsify the covering conjecture in a given dimension. By a recent result of Curtis McMullen the covering conjecture implies the Minkowski conjecture. Thus

(in principle) the Minkowski conjecture can be verified in a given dimension using our algorithm.

Appendix A: Polyhedral representation conversion. In Appendix A we provide some background on polyhedra and in particular on a fundamental problem in polyhedral combinatorics, on which many computational results described in this book rely: The representation conversion of polyhedra with large symmetries. We start with a brief review of some basic properties and explain how to compute different polyhedral symmetries. We address the group theoretical background as well as data structures and software tools, which are necessary to deal with large orbits. Finally, we describe Decomposition methods for the representation conversion problem, which have proved to perform best in practice on the polyhedra we treated during our studies.

Conclusions and prospects. In this book we describe foundations and some applications of a *Computational Geometry of Positive Definite Quadratic Forms*. Based on generalizations of Voronoi's reduction theories, we provide new algorithms and details on their practical implementation. So far, such implementations have only been used for applications in the context of lattice sphere coverings (see Chapter 5). However, we are convinced that many more, new results can be obtained. Some interesting possible future projects are listed in Appendix B.

We think in particular that (in analogy to the lattice covering problem) many new record breaking lattices for the packing-covering constant and for the so-called *quantizer problem* can be found. We strongly believe that the theory described in this book can be used to find periodic non-lattice sets, which are "better" (with respect to any of the discussed problems) than any lattice of the same dimension. We think that it is only a matter of time and a question of sufficient computational resources, until we will see a solution of the 6-dimensional covering and the 9-dimensional sphere packing problem.

A key ingredient for computational successes described in this book is the representation conversion of polyhedra under symmetry. We think that further improvement on the available tools will not only yield further progress for the problems discussed here, but also for applications beyond the scope of this book. Furthermore, we are convinced that the future will show more and more mathematical proofs based on rigorous numerical computations and non-linear convex optimization. However, there is still plenty of groundwork to be done.

So let's do it...

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Notations

In the following we list some of the notations used at different places of this book and which may not be commonly known (among mathematicians). The listing is in a mixed alphabetical (by initial sound) and thematic order. The second column lists the page of the first occurrence.

$\langle \cdot, \cdot \rangle$	2, 37	inner product on S^d or $S^{d,m}$
$\ \cdot \ $	5	Euclidean norm
Aut	33, 46, 92	autom. group of PQF, periodic form or Delone subdiv.
Aut_t	49	$\text{GL}_d^t(\mathbb{Z})$ -restricted automorphism group of PQF
B^d	5	Euclidean unit ball in \mathbb{R}^d
$\text{BR}_{L,\beta}(Q)$	86	matrix with property $ \text{BR}_{L,\beta}(Q) \geq 0 \Leftrightarrow \mu_L(Q) \leq \beta$
$\mathcal{B}_{L,\leq\beta}, \mathcal{B}_{L,=\beta}$	92	sets of PQFs with $\mu_L(Q) \leq \beta$ and $\mu_L(Q) = \beta$
$\text{cone}(M)$	29	conic hull of a set M
\mathbf{D}_α	92	set of PQFs Q with $\det Q \geq \alpha$
δ	7, 9, 38	packing density of discrete set, PQF or periodic form
δ_d	8	density of the densest lattice sphere packing in \mathbb{R}^d
$\delta_{d,m}$	38	density of the densest m -periodic sphere packing in \mathbb{R}^d
δ_d^*	9	density of the densest sphere packing in \mathbb{R}^d
det	6, 38	determinant of lattice, PQF (matrix) or periodic form
$\Delta(\mathcal{D})$	57, 60	secondary cone of Delone subdivision \mathcal{D}
$\Delta_T(\mathcal{D})$	67	T -secondary cone $\Delta(\mathcal{D}) \cap T$ with $T \subseteq S^d$ linear
$\Delta(\Lambda, P)$	74	secondary cone of a polyhedron P w.r.t. vertex-set Λ
dens Λ	10	point density of a discrete set Λ
$\text{Del}_\Lambda(Q)$	57	Delone subdivision of PQF Q w.r.t. vertex-set Λ
$\Gamma_d(N)$	46	principal congruence subgroup of level N
γ	13, 84	packing-covering constant of discrete set or PQF
γ_d	13	smallest lattice packing-covering constant in \mathbb{R}^d
γ_d^*	13	smallest packing-covering constant in \mathbb{R}^d
$\text{GL}_d(\mathbb{Z})$	2	$\{U \in \mathbb{Z}^{d \times d} : \det U = 1\}$

$\mathrm{GL}_d(\mathbb{R})$	4	$\{A \in \mathbb{R}^{d \times d} : \det A \neq 0\}$
$\mathrm{GL}_d^t(\mathbb{Z})$	46	automorphism group of standard periodic set Λ_t
$g_{L,\beta}$	94	gradient of smooth surface $\mathcal{B}_{L,=\beta}$
\mathcal{H}_d	6	Hermite's constant
$\lambda(L), \lambda(\Lambda)$	6, 9	packing radius of lattice or discrete set
$\lambda(Q), \lambda(X)$	3, 38	(generalized) arith. minimum of a PQF or periodic form
λ_i	21	i -th successive minimum of lattice or PQF
Λ_t	65	standard periodic vertex-set defined by t
$\mathcal{M}_d, \mathcal{M}_d^+$	19	Minkowski's reduction domains
$\mathrm{Min} Q, \mathrm{Min} X$	3, 38	representatives of (general.) arith. minimum $\lambda(Q), \lambda(X)$
$\mu(\Lambda)$	11	covering radius of discrete set Λ
$\mu(Q), \mu_\Lambda(Q)$	83, 84	inhom. minimum of PQF w.r.t. \mathbb{Z}^d , respectively Λ
$\mu_P(Q)$	86, 87	squared circumradius of P with respect to Q
$N_{V,\mathbf{w}}$	57	quadratic form defining regulator
$N_{L,L'}$	57	quadratic form def. regulator for adj. Del. simplices L, L'
$\mathcal{N}_{\Lambda,P}(Q)$	125	normal cone of Baranovskii cone $\Delta(\Lambda, P)$ at Q
$O_d(\mathbb{R})$	5	$\{O \in \mathbb{R}^{d \times d} : O^t O = \mathrm{id}_d\}$
$\mathcal{P}(Q), \mathcal{P}(X)$	31, 40	dual cones of (generalized) Voronoi domain $\mathcal{V}(Q), \mathcal{V}(X)$
\mathcal{P}_λ	27	Ryshkov polyhedron
$\mathcal{P}_{m,\lambda}$	38	generalized Ryshkov set
$\mathcal{P}_{\lambda,t}$	47	Ryshkov polyhedron of standard periodic set Λ_t
$p_{i,j,v}(X)$	38	polynomial $Q[t_i - t_j - v]$ for periodic form $X = (Q, t)$
\mathcal{S}^d	1	$\{Q \in \mathbb{R}^{d \times d} : Q^t = Q\}$
$\mathcal{S}_{>0}^d$	2	$\{Q \in \mathcal{S}^d : Q \text{ positive definite}\}$
$\mathcal{S}_{\geq 0}^d$	4	$\{Q \in \mathcal{S}^d : Q \text{ positive semi-definite}\}$
$\tilde{\mathcal{S}}_{\geq 0}^d$	35	rational closure of $\mathcal{S}_{>0}^d$
$\mathcal{S}_{>0}^{d,m}$	37	parameter space for m -periodic point sets in \mathbb{R}^d
$\mathcal{S}^{d,m}$	37	Euclidean space $\mathcal{S}^d \times \mathbb{R}^{d \times (m-1)}$ containing $\mathcal{S}_{>0}^{d,m}$
Θ	11, 83	covering density of discrete set or PQF
Θ_d	11	density of thinnest lattice covering in \mathbb{R}^d
Θ_d^*	11	density of thinnest covering in \mathbb{R}^d
Θ_P	123	covering density function of Delone polytope P
T_G	34	linear space of G -invariant quadratic forms
$\mathcal{V}(Q), \mathcal{V}(X)$	29, 40	(generalized) Voronoi domain
$\mathcal{W}_{\mathcal{D}, \leq \beta}$	92	set of PQFs in $\Delta(\mathcal{D})$ with $\mu(Q) \leq \beta$

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