High-dimensional polytopes defined by oracles: algorithms, computations and applications

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Abstract

The processing and analysis of high dimensional geometric data plays a fundamental role in disciplines of science and engineering. A systematic framework to study these problems has been developing in the research area of discrete and computational geometry. This Phd thesis studies problems in this area. The fundamental geometric objects of our study are high dimensional convex polytopes defined by an oracle.

The contribution of the thesis is threefold. First, the design and analysis of geometric algorithms for problems concerning high-dimensional convex polytopes, such as convex hull and volume computation and their applications to computational algebraic geometry and optimization. Second, the establishment of combinatorial characterization results for essential polytope families. Third, the implementation and experimental analysis of the proposed algorithms and methods.

Keywords: convex polytopes, volume computation, Newton polytope of sparse resultant, secondary polytope, regular triangulations, geometric predicates, algorithm engineering, experimental analysis

1 Introduction

The processing and analysis of high dimensional geometric data plays a fundamental role in disciplines of science and engineering. In the last decades many successful geometric algorithms have been developed in 2 and 3 dimensions. However, in most cases their performance in

*Dissertation advisor: Ioannis Z. Emiris, Professor higher dimensions is poor. This behaviour is commonly called *the curse of dimensionality*. A solution framework adopted for the healing of the curse of dimensionality is the exploitation of the special structure of the data, such as sparsity or low intrinsic dimension, and the design of approximation algorithms. This thesis studies problems inside this framework.

The main research area is discrete and computational geometry and its connections to branches of computer science and applied mathematics like polytope theory, algorithm engineering, randomized geometric algorithms, computational algebraic geometry and optimization. The fundamental geometric objects of the study are *polytopes*, with main properties of being *convex* and defined in a *high dimensional* space.

The contribution of this thesis is threefold. First, the design and analysis of geometric algorithms for problems concerning high-dimensional convex polytopes, such as convex hull and volume computation and their applications to computational algebraic geometry and optimization. Second, the establishment of combinatorial characterization results for essential polytope families. Third, the implementation and experimental analysis of the proposed algorithms and methods. The developed software is open-source, publicly available from:

`http://sourceforge.net/users/fisikop`.

It builds on, extends and is competitive with state-of-the-art geometric and algebraic software libraries such as `CGAL` [3] and `polymake` [17].

What follows is a brief presentation of the research topics and results of the thesis, avoiding technical details.

2 Polytopes and oracles

In polytope theory, a (convex) polytope P admits two explicit representations. The first is the set of P vertices, which is called the V-representation or vertex representation. The second is the bounded intersection of a set of linear inequalities or half-spaces, which is called

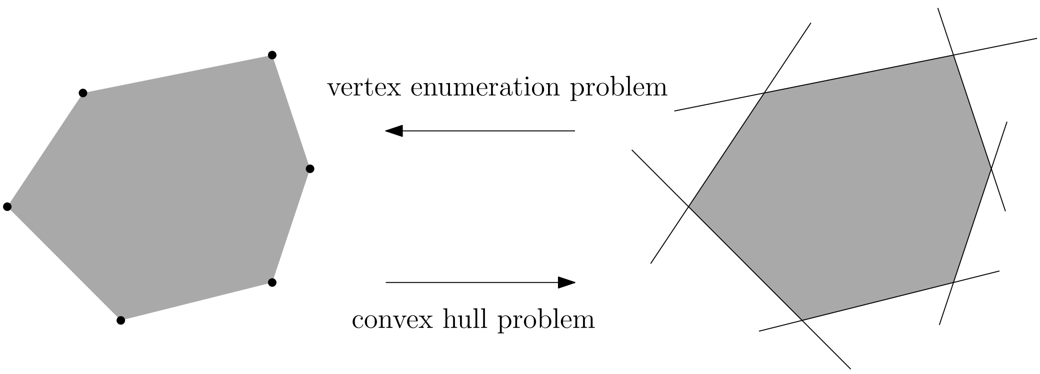
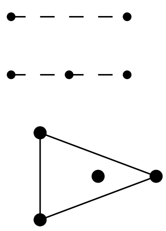


Figure 1: The V- and H-representation of a convex polygon.

H-representation or halfspace representation. Given a polytope in V-representation, computing the H-representation constitutes the *convex hull* problem, while the opposite is the *vertex enumeration* problem. These problems are algorithmically equivalent from a computational complexity point of view by *polytope duality* and establish two of the most important computational problems in discrete geometry. See Figure 1 for an illustration. For a detailed presentation on several aspects related to convex polytopes we refer to [26].

A polytope P can also be given by an implicit representation, called *(polytope) oracle*. An oracle is a black box routine that answers questions regarding P. An *optimization*, or *linear programming (LP)*, or *vertex* oracle given a vector c returns a vertex of P that has the maximum inner product with c among all points in P. Another important implicit representation for P is the *separation* oracle. That is, given a point x the oracle returns yes if $x \in P$ or a hyperplane that separates P from x otherwise. To illustrate the above definitions, let P be given in H-representation. Then an optimization oracle for P given a vector c solves an LP problem on P, while a separation oracle for P given point x evaluates the set of defining inequalities of P with x.

The relations among various oracles have been studied by Grötschel, Lovàsz and Schrijver in [20] by adopting the oracle Turing machine model of computation. To acquire, for example, an optimization oracle for P when P is given by a separation oracle, one has to solve a linear program over P. This can be done by the ellipsoid method [22]. Given an oracle for P, the entire polytope P can be reconstructed and



A_0 $\quad f_0(x) = ax^2 + b$

A_1 $\quad f_1(x) = cx^2 + dx + e$

$N(R)$ $\quad R(a,b,c,d,e) = ad^2b + c^2b^2 - 2caeb + a^2e^2$

Figure 2: The resultant of a system of two polynomials in one variable.

its explicit representation can be found using an incremental convex hull algorithm such as the Beneath-and-Beyond [4].

3 Algorithms for resultant polytopes

From the algebraic geometry perspective polytopes characterize polynomials better than total degree thus offering the fundamental representation in sparse elimination theory, called *Newton polytopes*. An important class of such polytopes is the Newton polytopes of the *sparse resultant polynomial* or simply the *resultant polytopes*. They have been studied by Gelfand, Kapranov and Zelevinsky in [19] and by Sturmfels in [25]. An example of the resultant of two polynomials f_0, f_1 in one variable x is depicted in Figure 2. It is a polynomial R in the coefficients a, b, c, d, e of the two polynomials which vanishes if the system we get by specializing a, b, c, d, e to numerical values has a solution. Here, the Newton polytope $N(R)$ of the resultant is a triangle.

In [19] the study of resultant polytopes is connected to the study of *secondary polytopes*. The secondary polytope of a pointset A is a fundamental object in geometric combinatorics since it offers a polytope realization of the graph of *regular triangulations* of the pointset. An equivalent realization is the graph of *regular fine mixed subdivisions* of the Minkowski sum of pointsets. Figure 3 depicts an example of secondary and resultant polytopes. In the special case where the points in A are in convex position and two dimensional all triangu-

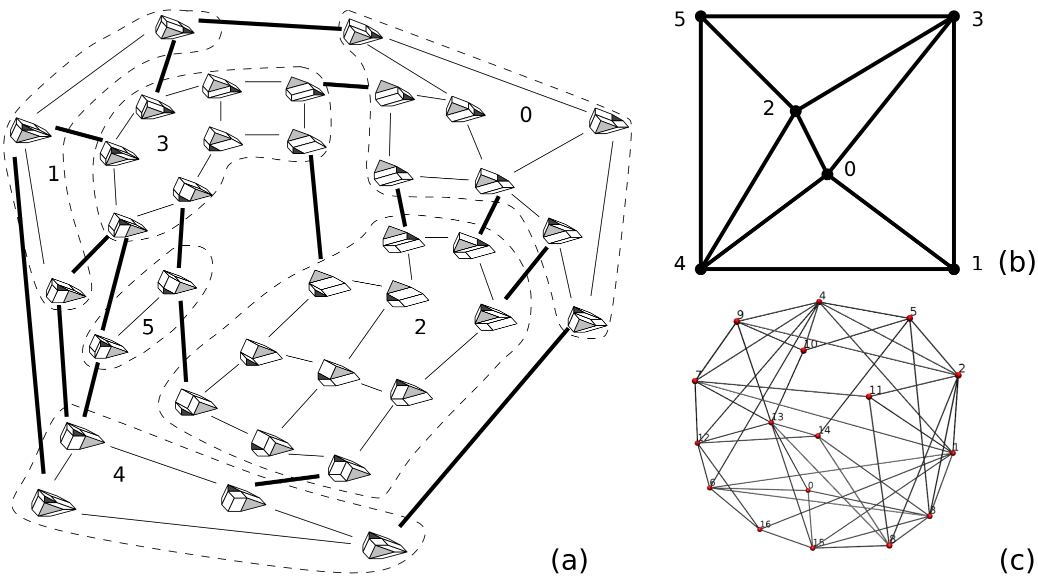


Figure 3: Example of secondary and resultant polytopes: (a) The secondary polytope of two triangles (dark, light grey) and one segment; vertices correspond to mixed subdivisions of the Minkowski sum $A_0 + A_1 + A_2$ and edges to flips between them (b) the resultant polytope, whose vertices correspond to the dashed classes of the secondary polytope. Bold edges of the secondary polytope map to edges of the resultant polytope (c) 4-dimensional resultant polytope of 3 generic trinomials with f-vector $(22, 66, 66, 22)$; figure made with `polymake`.

lations are regular and the secondary polytope is the 3-dimensional associahedron [24].

Chapter 2 of the thesis presents the design and the analysis of the first *output-sensitive* algorithm for computing (projections of) resultant polytopes. The algorithm is output-sensitive as it makes one oracle call per vertex and facet of the polytope. The key ingredients of that algorithm is the compact representation of resultant polytopes by an optimization oracle and the exploitation of their low intrinsic dimension. The oracle constructs regular triangulations in order to compute the optimal vertex in the polytope. Finally, the resultant polytope is reconstructed using an incremental convex hull algorithm that uses this oracle.

The algorithm is implemented in the software package `respol`, which computes 5-, 6- and 7-dimensional polytopes with $35{\cdot}10^3$, $23{\cdot}10^3$ and 500 vertices, respectively, within 2 hours on a standard computer, and the Newton polytopes of many important surface equations encountered in geometric modelling in $<$ 1sec, whereas the enumeration of the vertices of the corresponding secondary polytopes is intractable. `respol` has been used to solve essential problems in CAD [14] as well as to compute discriminant polynomials [15]. We propose and implement a technique called *hashing of determinants*, which avoids duplication of computations by exploiting the nature of determinants computed by the algorithm. In practice, this technique accelerates execution up to 100 times.

The results of this work have been published in [12] and their full version in [13]. An extension of the above method to computing discriminant polytopes is discussed in Section 2.6 and has appeared in [11].

4 Edge-skeleton computation

Motivated by the fact that the above algorithm is impractical in 8 or more dimensions since it relies on an incremental convex hull algorithm, the study extends in finding more efficient, i.e. *total polynomial time*, algorithms for convex hulls. An algorithm runs in total polynomial time if its time complexity is bounded by a polynomial in the input *and* output size. In general dimension finding a total polynomial time algorithm for vertex enumeration is a major open problem in algorithmic geometry. However, total polynomial time algorithms exist for vertex enumeration of special polytope cases, such as simplicial polytopes [1] and 0/1-polytopes [2].

Here we establish another case where total polynomial time algorithms exist. We present the first total polynomial time algorithm for a special case of the vertex enumeration problem where the polytope is given by an optimization oracle and we are also given a superset of its edge directions. In particular the algorithm computes the *edge-skeleton* (or 1-skeleton) of the polytope, which is the graph of polytope vertices and edges. Since the vertices are computed along with the skeleton, the edge-skeleton computation subsumes vertex enumeration.

We consider two main applications. We obtain total polynomial time algorithms for computing signed Minkowski sums of convex polytopes, where polytopes can be subtracted provided the signed sum is a convex polytope, and for computing secondary, resultant, and discriminant polytopes. Further applications include convex combinatorial optimization and convex integer programming, where we offer an alternative approach, thus removing the exponential dependence on the dimension in the complexity.

The results of this work are presented in Chapter 3 of the thesis. Some preliminary results have been published in [9] and their full version in [10].

5 Approximate volume computation

Vertex enumeration in high dimensions (e.g. one hundred) using the above methods is a futile attempt. Thus, this thesis aims at exploiting the limits of learning fundamental characteristics of a polytope such as its volume. Although volume computation is #-P hard for V- and H-representations of polytopes [7] there exist randomized polynomial time algorithms to approximate the volume of a convex body with high probability and arbitrarily small relative error. Starting with the breakthrough polynomial time algorithm of [6], subsequent results brought down the exponent on the dimension from 27 to 4 [23]. However, the question of an efficient implementation had remained open.

This thesis undertakes this by experimentally studying the fundamental problem of computing the volume of a convex polytope given as an intersection of linear inequalities. We implement and evaluate practical randomized algorithms for accurately approximating the polytope's volume in high dimensions (e.g. one hundred). To carry out this efficiently we experimentally correlate the effect of parameters, such as random walk length and number of sample points, on accuracy and runtime. Moreover, we exploit the problem's geometry by implementing an iterative rounding procedure, computing partial generations of random points and designing fast polytope boundary oracles. Our publicly available code is significantly faster than exact computation. We provide volume estimations for the Birkhoff polytopes $B_{11}, \dots, B_{15}$, whereas only the volume of B_{10} has computed exactly.

The results of this work are presented in Chapter 4 of the thesis and published in [8].

6 Combinatorics of resultant polytopes

We study the combinatorics of resultant polytopes. These are known in the case of two polynomials in one variable, also known as the Sylvester case [18] and in the case where the polytope's dimension is up to 3 [25]. We extend this work and at the same time answer an open question raised in [21] by studying the combinatorial characterization of 4-dimensional resultant polytopes, which show a greater diversity and involve computational and combinatorial challenges.

In particular, our experiments, based on `respol`, provide a series of polytopes that establish lower bounds on the maximal number of faces. By studying subdivisions of Minkowski sums, called *mixed subdivisions*, we obtain tight upper bounds on the maximal number of facets and ridges. These yield an upper bound for the number of vertices, which is 28 whereas the general bound yields 6608 [25]. Figure 3(c) shows an instance with f-vector $(22, 66, 66, 22)$ that maximizes the number of facets and ridges.

We establish a result of independent interest, namely that the f-vector is maximized when the input is sufficiently generic, namely full dimensional and without parallel edges. Lastly, we offer a classification result of all possible 4-dimensional resultant polytopes.

The results of this work are presented in Chapter 5 of the thesis and have been published in [5].

7 Geometric predicates

Geometric algorithms involve both combinatorial and algebraic computation. In many cases, such as convex hull computations, the later boils down to determinant sign computations, also called *geometric predicates*. As the dimension of the computation space grows, a higher percentage of the computation time is consumed by these predicates. Our goal is to study the sequences of determinants that appear in geometric algorithms. We use dynamic determinant algorithms to speed-up the computation of each predicate by using information from previously computed predicates.

We propose two dynamic determinant algorithms with quadratic complexity when employed in convex hull computations, and with linear complexity when used in point location problems. Moreover, we implement them and perform an experimental analysis. Our implementations outperform the state-of-the-art determinant and convex hull implementations in most of the tested scenarios, as well as giving a speed-up of 78 times in point location problems.

The results of this work are presented in Chapter 6 of the thesis and have been published in [16]. The developed software package has been submitted in `CGAL` [3] and is currently under revision.

8 Extensions and open problems

Several intriguing open questions emerge by the study of this thesis. From the geometric combinatorics point of view one question is to understand the symmetry of the maximal f-vector, i.e. vector of polytope's face cardinalities, that appear in the study of the combinatorics of 4-dimensional resultant polytopes.

There are a few questions related to sampling. The first is to study volume approximation algorithms when an optimization oracle is available. The current research focuses on convex bodies, or polytopes, represented by a membership oracle. A special case which is also interesting is to sample random points from polytopes given in V-representation without using membership queries. Other related problems are computing the volume of spectahedra or general semi-algebraic sets, application of the current software to other #P-hard problems like counting linear extensions of partial ordered sets, integration of polynomial functions over convex polytopes, study polytopes that are easy/difficult to sample from under the assumption that they are rounded, study the quality of sampling or compare point samples, and sampling integer points from polytopes.

Nearest neighbour searching has been considered as one of the most fundamental problems in computer science. Our study in Chapter 4 paves the way for an application of approximate nearest neighbour searching to approximate polytope oracles and polytope volume approximation.

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