How to Integrate a Polynomial over a Convex Polytope: Combinatorics and Algorithms

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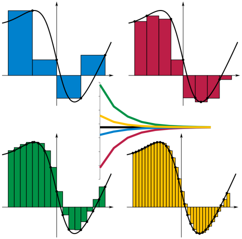
Theorems are joint work with

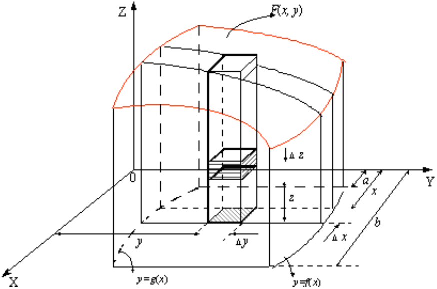
Software **LattE integrale** was developed with help by several smart students. Most notably

Our Problem
Background and Motivation

Our Wishes

Given P be a d-dimensional rational polytope inside $\mathbb{R}^n$ and let $f \in \mathbb{Q}[x_1, \ldots, x_n]$ be a polynomial with rational coefficients.





Compute the EXACT value of the integral $\int_P f \; dm$?

Example

If we integrate the monomial $x^{17}y^{111}z^{13}$ over the three-dimensional standard simplex Δ. Then $\int_\Delta x^{17}y^{111}z^{23}dxdydz$ equals exactly

$$\frac{1}{3176663991373060176558829070734899482827062815673600000}$$

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- **Tomography and Inverse problems:** The X-rays of a polytope can be used to estimate the moments of the underlying mass distribution. One can reconstruct of any convex polytope, from knowledge of its moments.
- **Probability and Statistics:** marginal likelihood integrals in model selection.
- But, why EXACT integration? Numeric Integration is successful, right? **My point:**Exact integration useful for calibration!!!!

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- (for computational algebraic geometers) Let $f_1, \ldots, f_n$ be polynomials in $\mathbb{C}[x_1, \ldots, x_n]$. Let $New(f_j)$ denote the Newton polytope of f_j, If $f_1, \ldots, f_n$ are generic, then the number of solutions of the polynomial system of equations $f_1 = 0, \ldots, f_n = 0$ with no $x_i = 0$ is equal to the normalized mixed volume $n! MV(New(f_1), \ldots, New(f_n))$.

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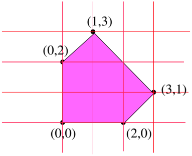
- (for Combinatorialists) Volumes count things! $CR_m = \{(a_{ij}) : \sum_i a_{ij} = 1, \sum_j a_{ij} = 1,$ with $a_{ij} \geq 0$ but $a_{ij} = 0$ when $j > i+1$ $\}$, then $NV(CR_m) =$ product of first $(m-2)$ Cat alan numbers. (D. Zeilberger).
- Many Other applications...

A running example

Suppose we wish to integrate $\int_{pentagon} f(x,y)dxdy$



We teach undergraduates to decompose the integral into boxes:

$$\int_0^1 \int_0^{x+2} f(x,y)dydx + \int_1^2 \int_0^{-x+4} f(x,y)dydx + \int_2^3 \int_{x-2}^{-x+4} f(x,y)dydx$$

Hey! I took calculus already!!

For $f(\mathbf{x}) = f(x_1, \ldots, x_d)$ a polynomial function calculus books say THINK BOXES, ITERATION!!!

For a full-dimensional polytope $P = \{ A\mathbf{x} \leq \mathbf{b} \} \subseteq \mathbb{R}^d$

$$\int_P f(\mathbf{x}) d\mathbf{x} = \sum_{boxes} \int_{a_1}^{b_1} \int_{a_2(x_1)}^{b_2(x_1)} \int_{a_3(x_1,x_2)}^{b_3(x_1,x_2)} \ldots \int_{a_d(x_1,\ldots,x_{d-1})}^{b_d(x_1,\ldots,x_{d-1})} f(\mathbf{x}) d\mathbf{x}$$

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M. Schechter, American Mathematical Monthly **105** (1998), 246–251.

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To handle the parametric limits of integration: Need Fourier–Motzkin projection – exponential time

BAD even for simplices

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- Even deterministic is already hard, but randomized approximation can be done efficiently (Barany, Dyer, Elekes, Furedi, Frieze, Kannan, Lovász, Rademacher, Simonovits, Vempala, others)

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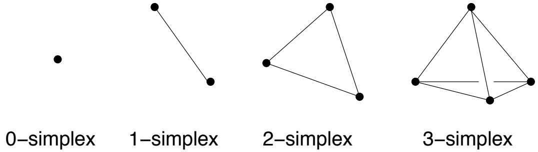

A d-simplex has exactly $\binom{d+1}{i+1}$ faces of dimension i, $(i = -1, 0, \ldots, d)$, which are themselves i-simplices.
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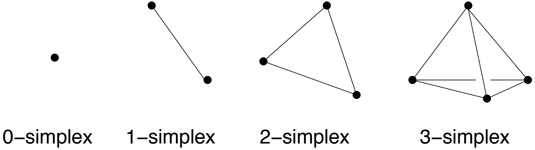

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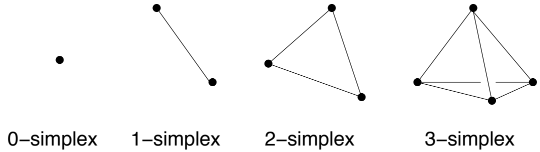

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- To compute the integral of a polytope: divide it as a disjoint union of simplices, calculate integral for each simplex and then add them up!
- **Remark:** Computing volume and centroids of simplices can be done efficiently! We generalize these facts.

Our Results

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TECHNICAL REMARKS: Non-full-dimensional OK!

For calculations we work with the *integral Lebesgue measure* $\mathfrak{d}m$:

- When the polytope P is of full dimension n, in $\mathbb{R}^n$ $\mathfrak{d}m$ is the standard Lebesgue measure, which gives volume 1 to the fundamental domain of the lattice $\mathbb{Z}^n$.

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- For this $\mathfrak{d}m$, every integral of a polynomial function with rational coefficients will be a *rational number*. **Example:** the diagonal of the unit square has length 1 instead of $\sqrt{2}$.

BAD news: Integration of arbitrary polynomials over simplices is NP-hard

- The clique problem (does G contain a clique of size $\geq n$) is NP-complete. (Karp 1972).
- **Theorem** [Motzkin-Straus 1965]
  G a graph with clique number $\omega(G)$.
  $Q_G(x) := \frac{1}{2}\sum_{(i,j)\in E(G)} x_i x_j$. Function on standard simplex in $\mathbb{R}^{|V(G)|}$.
  Then $\|Q_G\|_\infty = \frac{1}{2}(1 - \frac{1}{\omega(G)})$.
- **Lemma** Let G a graph with d vertices. The clique number $\omega(G)$ is equal to $\left\lceil \frac{1}{1-2\|Q_G\|_p} \right\rceil$. ($L^p$-norm, Holder inequality) as long as $p \geq 4(e-1)d^3 \ln(32d^2)$, the

GOOD News: Fast Integration for powers of linear forms

Theorem: There exists a polynomial-time algorithm that given an integer M, a linear form $\langle \ell, x \rangle$, and a simplex Δ with vertices $\mathbf{s}_1, \ldots, \mathbf{s}_{d+1} \in \mathbb{Q}^d$ computes the integral

$$\int_\Delta \langle \ell, \mathbf{x} \rangle^M \mathfrak{d}m$$

.

When ℓ is regular, w.r.t. Δ, i.e., $\langle \ell, \mathbf{s}_i \rangle \neq \langle \ell, \mathbf{s}_j \rangle$ for any pair $i \neq j$. Then answer has a **short sum of rational functions** on ℓ_i.

COOL formula for the integral of power of linear forms

Theorem Let Δ be a simplex. Let ℓ be a linear form which is regular w.r.t. Δ, i.e., $\langle \ell, \mathbf{s}_i \rangle \neq \langle \ell, \mathbf{s}_j \rangle$ for any pair $i \neq j$. Then

$$\int_{\Delta} < \ell, x >^{M} \mathfrak{d}m = d! \operatorname{vol}(\Delta, \mathfrak{d}m) \frac{M!}{(M+d)!} \Big(\sum_{i=1}^{d+1} \frac{\langle \ell, \mathbf{s}_i \rangle^{M+d}}{\prod_{j \neq i} \langle \ell, \mathbf{s}_i - \mathbf{s}_j \rangle} \Big).$$

Two beautiful formulas (for fixed degree M):

Theorem Let Δ be the simplex that is the convex hull of $\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_{d+1}$ in $\mathbb{R}^n$, and let ℓ be an arbitrary linear form on $\mathbb{R}^n$. Then

$$\int_\Delta \ell^M \mathfrak{d}m = d!\,\mathrm{vol}(\Delta, \mathfrak{d}m) \frac{M!}{(M+d)!} \sum_{\mathbf{k} \in \mathbb{N}^{d+1}, |\mathbf{k}|=M} \langle \ell, \mathbf{s}_1 \rangle^{k_1} \cdots \langle \ell, \mathbf{s}_{d+1} \rangle^{k_{d+1}}. \tag{1}$$

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If H is a symmetric multilinear form defined on $(\mathbb{R}^d)^M$. Then one has

$$\int_\Delta H(\mathbf{x}, \mathbf{x}, \dots, \mathbf{x}) d\mathbf{x} = \frac{\mathrm{vol}(\Delta)}{\binom{M+d}{M}} \sum_{1 \le i_1 \le i_2 \le \cdots i_M \le d+1} H(\mathbf{s}_{i_1}, \mathbf{s}_{i_2}, \dots, \mathbf{s}_{i_M}). \tag{2}$$

We can apply this to ALL polynomials!!

- We can compute integrals of **arbitrary** polynomials too!
- **Lemma:** Write any monomial of degree M as a sum of powers of linear forms (at most 2^M terms):

$$x_1^{m_1} x_2^{m_2} \cdots x_d^{m_d} = \frac{1}{|m|!} \sum_{0 \le p_i \le m_i} (-1)^{|m|-|p|} \binom{m_1}{p_1} \cdots \binom{m_d}{p_d} (p_1 x_1 + \cdots + p_d x_d)^{|m|}.$$

- **Example:**

$$7x^2 + y^2 + 5z2 + 2xy + 9yz =$$

$$\frac{1}{8}(12(2x)^2 - 9(2y)^2 + (2z)^2 2 + 8(x+y)^2 + 36(y+z)^2)$$

More good news: Polynomials of fixed degree

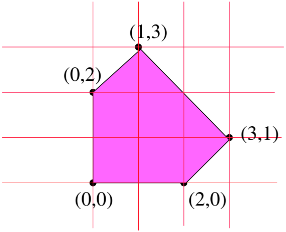
Corollary: For each fixed number $M \in \mathbb{N}$, there exists a polynomial-time algorithm for the problem: **Input:**

- numbers $d, n \in \mathbb{N}$
- affinely independent rational vectors $\mathbf{s}_1, \ldots, \mathbf{s}_{d+1} \in \mathbb{Q}^n$ in binary encoding,
- a polynomial $f \in \mathbb{Q}[x_1, \ldots, x_n]$ of degree at most M,

Output: in binary encoding: the rational number $\int_\Delta f(\mathbf{x}) \mathfrak{d}m$,

Running Example CONTINUES

- Integrate $\int_{pentagon} (c_1 x + c_2 y)^M dxdy$



- The answer is a rational function:

$$\frac{M!}{(M+2)!}\left(\frac{(2\,c_1)^{M+2}}{c_1(-c_1-c_2)} + 4\,\frac{(3\,c_1+c_2)^{M+2}}{(c_1+c_2)(2\,c_1-2\,c_2)} + 4\,\frac{(c_1+3\,c_2)^{M+2}}{(c_1+c_2)(-2\,c_1+2\,c_2)} + \frac{(2\,c_2)^{M+2}}{(-c_1-c_2)c_2}\right)$$

- When $M = 0$ we are computing the AREA of the pentagon: The rational function simplifies to a number!! Indeed area is 6 because:

$$12 = 4\,\frac{c_1}{-c_1-c_2} + 4\,\frac{(3\,c_1+c_2)^2}{(c_1+c_2)(2\,c_1-2\,c_2)} + 4\,\frac{(c_1+3\,c_2)^2}{(c_1+c_2)(-2\,c_1+2\,c_2)} + 4\,\frac{c_2}{-c_1-c_2}$$

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- For any M when (c_1, c_2) is not perpendicular to any of the edge directions we simply plug in numbers.
  For instance for $M = 100$ and $(c_1 = 3, c_2 = 5)$:
  $$\frac{22727636938689966389358886740322023383316784295938226547419458531150195170448158078285549739919811}{1717}$$

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- Else we have to compute some complex residues, because there are resolvable singularities (this is true for only a few linear forms in the universe!).
- We have implemented TWO different algorithms in LattE Integrale!

Our Methods:

A classical notion: Valuations

- A **valuation** on polyhedra is a linear map from the vector space of characteristic functions $\chi(\mathfrak{p}_i)$ of polyhedra into a field.

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- **Example:**

$$\chi(\mathfrak{p}_1 \cup p_2) + \chi(\mathfrak{p}_1 \cap p_2) - \chi(\mathfrak{p}_1) - \chi(\mathfrak{p}_2) = 0,$$

An exponential integral valuation for polyhedra

$\mathfrak{p}$ (convex) rational polyhedron. Define

$$I(\mathfrak{p})(\xi) := \int_{\mathfrak{p}} e^{\langle \xi, x \rangle} \, dm$$

when the integral converges.

Lemma If $\mathfrak{p}$ contains a line, then set $I(\mathfrak{p}) := 0$.

Valuations for simplicial cones

Theorem: $s+\mathfrak{c}$ affine cone with vertex s and integral generators $v_1, \ldots, v_d \in$ lattice Λ. Thus $\mathfrak{c} = \mathbb{R}_+ v_1 + \ldots \mathbb{R}_+ v_d$.
The exponential integral valuation takes the form:

$$I(s+\mathfrak{c})(\xi) = |\det_{\Lambda}(v_j)| \prod_j \frac{-e^{\langle \xi, s\rangle}}{\langle \xi, v_j\rangle}$$

where $\mathfrak{b} = \sum_j [0,1[v_j$, *semi-closed cell.*

EXAMPLE: $I(\mathfrak{p})$ in dimension one

For the line segment $[a, b]$ we have:

$$\chi([a, b]) = \chi([-\infty, b]) + \chi([a, +\infty]) - \chi(\mathbb{R})$$

Apply exponential integral valuation to this identity.

$$I([a, b]) = I([-\infty, b]) + I([a, +\infty]) - I(\mathbb{R})$$

By the properties we discussed yields the desired answer $e^b - e^a$.

Polyhedron $\equiv$ sum of its supporting cones at vertices

Theorem *(Brion-Lawrence-Varchenko)*
$\mathfrak{p}$ convex polyhedron, $s + \mathfrak{c}_s$ supporting cone at vertex s.

$$S(\mathfrak{p}) = \sum_{s \in \text{ vertices}} S(s + \mathfrak{c}_s), \quad I(\mathfrak{p}) = \sum_s I(s + \mathfrak{c}_s)$$

Polyhedron $\equiv$ sum of its supporting cones at vertices

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Corollary: Let Δ be a simplex. Let ℓ be a linear form which is regular w.r.t. Δ, i.e., $\langle \ell, \mathbf{s}_i \rangle \neq \langle \ell, \mathbf{s}_j \rangle$ for any pair $i \neq j$. Then

$$\int_\Delta e^{<\ell, x>} \mathfrak{d}m = d! \operatorname{vol}(\Delta, \mathfrak{d}m) \sum_{i=1}^{d+1} \frac{e^{\langle \ell, \mathbf{s}_i \rangle}}{\prod_{j \neq i} \langle \ell, \mathbf{s}_i - \mathbf{s}_j \rangle}.$$

From Exponentials to Powers of Linear Forms

- To compute $L^M(P)(\ell) = \int_P \langle \ell, x \rangle^M \mathfrak{d}m$ for linear form ℓ such that the integral exists over a polytope P we use valuation property and do it for cones:

$$\int_{s+C} e^{\langle t\ell, x \rangle} \mathfrak{d}m = \mathrm{vol}(\Pi_C) e^{\langle t\ell, s \rangle} \prod_{i=1}^{d} \frac{1}{\langle -t\ell, u_i \rangle}. \qquad (3)$$

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- We equate it to the **Laurent series expansion** around $t = 0$ of the right-hand-side expression, which is a meromorphic function of t.

$$\mathrm{vol}(\Pi_C)e^{\langle t\ell,s\rangle}\prod_{i=1}^{d}\frac{1}{\langle -t\ell u_i\rangle}=\sum_{n=0}^{\infty}t^{n-d}\frac{\langle \ell,s\rangle^n}{n!}\cdot\mathrm{vol}(\Pi_C)\prod_{i=1}^{d}\frac{1}{\langle -\ell,u_i\rangle},$$

thus we can conclude the following.

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Corollary

For a regular linear form ℓ, a simplicial cone C generated by rays $u_1, u_2, \ldots u_d$ with vertex s

$$\int_{s+C} \langle \ell, x\rangle^M \mathfrak{d}m = \frac{M!}{(M+d)!} \mathrm{vol}(\Pi_C) \frac{(\langle \ell, s\rangle)^{M+d}}{\prod_{i=1}^{d} \langle -\ell, u_i\rangle}. \qquad (4)$$

Corollary

If $\langle -\ell, u_i\rangle = 0$ *for some* u_i, *then*

$$\int_{s+C} \langle \ell, x\rangle^M \mathfrak{d}m = \frac{M!}{(M+d)!}\,\mathrm{vol}(\Pi_C)\,\mathrm{Res}_{\epsilon=0}\,\frac{(\langle \ell+\hat{\epsilon}, s\rangle)^{M+d}}{\epsilon \prod_{i=1}^{d}\langle -\hat{\ell}-\hat{\epsilon}, u_i\rangle},$$

where $\hat{\epsilon}$ *is a vector in terms of* ϵ *such that* $\langle -\ell - \hat{\epsilon}, u_i\rangle \neq 0$ *for all* u_i,

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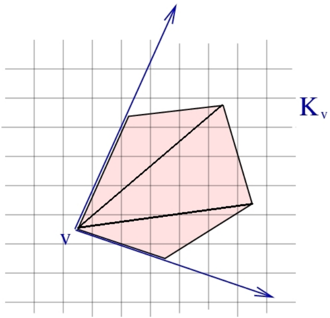
Corollary

For any triangulation $\mathcal{D}_s$ *of the feasible cone* C_s *at each of the vertices* s *of the polytope* P *we have*

$$\int_P \langle \ell, x \rangle^M \mathfrak{d}m = \sum_{s \in V(P)} \sum_{C \in \mathcal{D}_s} \int_{s+C_s} \langle \ell, x \rangle^M$$

TWO MAIN OPTIONS



Triangulate the polytope and integrate simplex-by-simplex OR iintegrate cone-by-cone

CONCLUSIONS

- Our work generalizes prior work by Jim Lawrence on volume computation and it gives algorithmic versions of results by Brion, Barvinok, Lasserre, Varchenko, and others.

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- Integration of polynomials of fixed degree is efficient too, but integration of arbitrary powers of quadratic forms is NP-hard.
- Algorithms run nicely in practice!!! Download the new **LattE integrale!**

Quick history of LattE

Figure: The new LattE includes integration.

- 2001 (De Loera et al.): LattE was developed as a software tool to count l attice points in integer polytopes through generating functions as its data structures.
- 2007 (Köppe): LattE macchiato (new algorithms and improved implementation)
- 2011: LattE integrale now includes volume computation and integration of polynomials over polytopes.
- The current team includes JDL, B. Dutra, and M. Köppe.

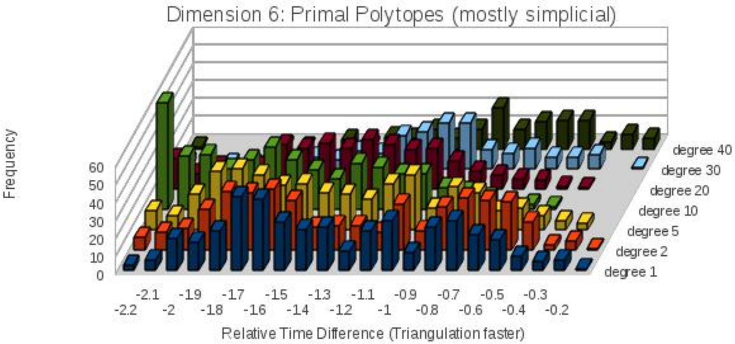
Experiments

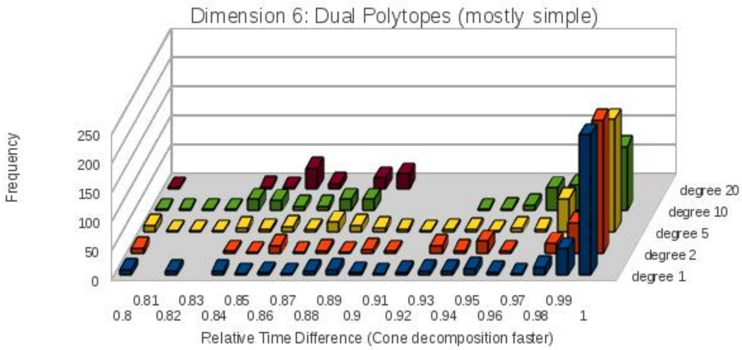
Table: Average and standard deviation of integration time in seconds of a random monomial of prescribed degree by decomposition into linear forms over a d-simplex (average over 50 random forms)

	Degree										
d	1	2	5	10	20	30	40	50	100	200	300
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	1.0	3.8
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.4	1.7
3	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	2.3	38.7	162.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	1.4	24.2	130.7
4	0.0	0.0	0.0	0.0	0.0	0.1	0.4	0.7	22.1	–	–
	0.0	0.0	0.0	0.0	0.0	0.1	0.3	0.7	16.7	–	–
5	0.0	0.0	0.0	0.0	0.1	0.3	1.6	4.4	–	–	–
	0.0	0.0	0.0	0.0	0.0	0.2	1.3	3.5	–	–	–
6	0.0	0.0	0.0	0.0	0.1	1.1	4.7	15.6	–	–	–
	0.0	0.0	0.0	0.0	0.1	1.0	4.3	14.2	–	–	–
7	0.0	0.0	0.0	0.0	0.2	2.2	12.3	63.2	–	–	–
	0.0	0.0	0.0	0.0	0.2	1.7	12.6	66.9	–	–	–
8	0.0	0.0	0.0	0.0	0.4	4.2	30.6	141.4	–	–	–
	0.0	0.0	0.0	0.0	0.3	3.0	31.8	127.6	–	–	–
10	0.0	0.0	0.0	0.0	1.3	19.6	–	–	–	–	–
	0.0	0.0	0.0	0.0	1.4	19.4	–	–	–	–	–
15	0.0	0.0	0.0	0.1	5.7	–	–	–	–	–	–
	0.0	0.0	0.0	0.0	3.6	–	–	–	–	–	–
20	0.0	0.0	0.0	0.2	23.3	–	–	–	–	–	–
	0.0	0.0	0.0	1.3	164.8	–	–	–	–	–	–

Comparing the triangulation and cone-decomposition methods

Shown: Relative time difference between over random polytopes in dimension 6.




Dimension 6: Dual Polytopes (mostly simple)
Frequency
250
200
150
100
50
0
0.81 0.83 0.85 0.87 0.89 0.91 0.93 0.95 0.97 0.99
0.8 0.82 0.84 0.86 0.88 0.9 0.92 0.94 0.96 0.98 1
Relative Time Difference (Cone decomposition faster)
degree 20
degree 10
degree 5
degree 2
degree 1

Thank you!