The generating function approach to mixed-integer nonlinear optimization

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based on joint work with

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J. A. De Loera, M. Vergne, Y. Zhou

(and earlier joint work with J. A. De Loera, R. Hemmecke, R. Weismantel)

The framework: The summation method for optimization

A.I. Barvinok, *Exponential integrals and sums over convex polyhedra*, Funktsional. Anal. i Prilozhen. 26 (1992).
J.B. Lasserre, *Generating functions and duality for integer programs*, Discrete Optim. 1 (2004).
De Loera, Hemmecke, **Kö.**, Weismantel, Mathematics of Operations Research, **31** (2006), pp. 147–153
J.B. Lasserre, *Linear and Integer Programming vs Linear Integration and Counting*, Springer, 2009

Maximization of a non-negative function f over a feasible region F is "just" the limit case of power-p integration (summation):

$$\lim_{p\to\infty} ||f||_{p,F} = ||f||_{\infty,F}$$

With

- $f \in \mathbf{Q}[x_1,\dots,x_d]$ a non-negative polynomial, $g := f^p$,
- $F = P$ a polytope or $F = P \cap \mathbf{Z}^d$ or $F = P \cap (\mathbf{Z}^{d_1} \times \mathbf{R}^{d_2})$

this leads to studying:

Problem of exact integration

Given a polytope $P \subseteq \mathbf{R}^n$ and a polynomial $g \in \mathbf{Q}[x_1,\dots,x_n]$, compute the integral

$$\int_P g(\mathbf{x})\,\mathrm{d}\mathbf{x}.$$

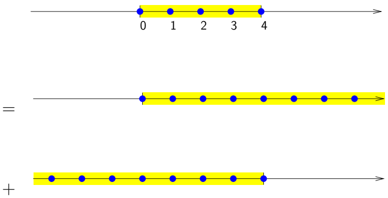
Problem of exact summation

Given a polytope $P \subseteq \mathbf{R}^d$ and a polynomial $g \in \mathbf{Q}[x_1,\dots,x_d]$, compute the discrete sum

$$\sum_{x\in P\cap\mathbf{Z}^d} g(\mathbf{x})$$

...

Summation of polynomial densities with the Euler differential operator



$$S(z) = z^0 + z^1 + z^2 + z^3 + z^4 = \frac{1}{1-z} - \frac{z^5}{1-z}$$

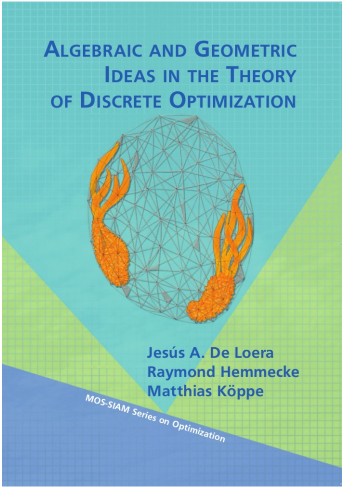
Apply differential operator:

$$\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right) S(z) = \color{red}{1}z^1 + \color{red}{2}z^2 + \color{red}{3}z^3 + \color{red}{4}z^4 = \frac{1}{(1-z)^2} - \frac{-4z^5 + 5z^4}{(1-z)^2}$$

Apply differential operator again:

$$\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right) S(z) = \color{red}{1}z^1 + \color{red}{4}z^2 + \color{red}{9}z^3 + \color{red}{16}z^4 = \frac{z + z^2}{(1-z)^{\color{blue}{3}}} - \frac{25z^5 - 39z^6 + 16z^7}{(1-z)^{\color{blue}{3}}}$$

Commercial break



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Two bounds: primal and dual (discrete case)

Consider the (discrete) optimization problem $\max\{\, f(\mathbf{x}) : \mathbf{x} \in F \,\}$ where f is non-negative on F and the feasible region F is finite.

Approximation properties of ℓ_p norms (Hölder)

$$F = \{\mathbf{x}^1, \dots, \mathbf{x}^N\} \qquad \text{and} \qquad \mathbf{f} = \begin{pmatrix} f(\mathbf{x}^1) \\ \vdots \\ f(\mathbf{x}^N) \end{pmatrix} \in \mathbf{R}^N.$$

Dual bound (upper bound on maximum value):

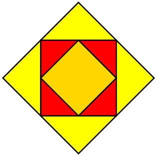
$$\|\mathbf{f}\|_\infty \leq \|\mathbf{f}\|_p =: U_p$$

Primal bound (lower bound on maximum value):

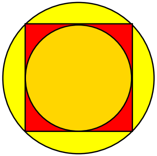
$$L_p := N^{-1/p}\, \|\mathbf{f}\|_p = \frac{\|\mathbf{f}\|_p}{\|\mathbf{1}\|_p} \leq \|\mathbf{f}\|_\infty$$

(both bounds converge to $\|\mathbf{f}\|_\infty$, oblivious to properties of f)

$k = 1$



$k = 2$



Continuous case: Use properties of f, e.g., a Lipschitz constant.

Integer polynomial optimization – Analysis in fixed dimension

De Loera, Hemmecke, **Kö.**, Weismantel, Mathematics of Operations Research, **31** (2006), pp. 147–153
De Loera, Hemmecke, **Kö.**, Weismantel, *Math. Prog.* 2008

Fix d.

- Linear f can be optimized in polynomial time (Lenstra, 1983)
- Convex polynomial f can be minimized in polynomial time (Khachiyan–Porkolab, 2000)
- Optimizing an arbitrary degree-4 polynomial f for $d = 2$ is NP-hard

Theorem (Fully Polynomial-Time Approximation Scheme, FPTAS)

For every $\epsilon > 0$, there exists an algorithm $\mathcal{A}_\epsilon$ for non-negative f with running time polynomial in the input size and $1/\epsilon$, which computes an approximation $\mathbf{x}_\epsilon \in P \cap \mathbf{Z}^d$ with

$$|f(\mathbf{x}_\epsilon) - f(\mathbf{x}^{\max})| \leq \epsilon f(\mathbf{x}^{\max}).$$

"Weak" ("Range-relative") FPTAS for Integer Optimization

... for arbitrary f ... computes a solution $\mathbf{x}_\epsilon \in P \cap \mathbf{Z}^d$ with

$$\left|f(\mathbf{x}_\epsilon) - f(\mathbf{x}^{\max})\right| \leq \epsilon \left|f(\mathbf{x}^{\max}) - f(\mathbf{x}^{\min})\right|.$$

Via discretization: FPTAS for fixed number of integer and continuous variables.

Computational experiments – quality of the discrete primal, dual bounds

Ongoing experiments by Ph.D. student Brandon Dutra, with J.A. De Loera

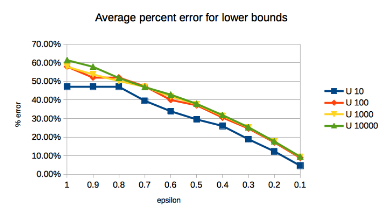
Inspired by the preprint:

- C. Buchheim and C. D'Ambrosio, Box-constrained mixed-integer polynomial optimization using separable underestimators, 2013,

we consider separable polynomial functions over box domains.

- If $f \geq 0$ on F, if $p = \left\lceil (1 + \frac{1}{\epsilon}) \log N \right\rceil$, then L_p is a $(1-\epsilon)$-approximation, U_p a $(1+\epsilon)$-approximation to $f_{\max}$.
- Consider the box domains $[-M, M]^{20}$ for $M = 10$, $M = 100$, $M = 1000$, $M = 10000$.
- Draw ten random homogeneous degree-4 separable polynomials f in 20 variables.
- Apply a range-approximating shifting trick to make $f + s \geq 0$.

Plot the actual approximation error of primal (lower) bounds L_p for different prescribed ϵ values.



The actual approximation error for the dual (upper) bounds U_p is much lower.

Even with $\epsilon = 1$ the percent error is $< 1\%$ for $M \geq 100$.

The $[-10, 10]^{20}$ box starts at 6%.

Computational experiments – computation time of the bounds

Ongoing experiments by Ph.D. student Brandon Dutra, with J.A. De Loera

The table below show the average time in seconds needed to compute the upper and lower bounds.

	Average computation time (CPU seconds)				
M	$\epsilon = 0.9$	$\epsilon = 0.7$	$\epsilon = 0.5$	$\epsilon = 0.3$	$\epsilon = 0.1$
10	0.14	0.20	0.48	1.46	30.34
100	0.96	1.34	2.60	7.54	271.76
1000	2.68	3.88	7.40	26.66	1426.20
10000	6.14	10.46	21.16	82.14	4182.74

(Preliminary implementation in LattE integrale.)

V. Baldoni, N. Berline, J.A. De Loera, B. Dutra, **Kö.**, M. Vergne: LattE integrale with top Ehrhart, version 1.6, Sept. 2013.

http://www.math.ucdavis.edu/~latte/

Image source: Wikipedia

Intermediate sums and mixed-integer optimization

The idea to use intermediate sums appeared first in Barvinok (2006), for the computation of the top k Ehrhart coefficients of a rational simplex in varying dimension. We take them to the generating-function (Laplace-transform) level and use them for mixed-integer optimization.

Theorem (S^L version of the Khovanskii–Pukhlikov theorem)

Let $L \subseteq V$ be a rational subspace. There exists a unique valuation S^L which to every rational polyhedron $P \subset V$ associates a meromorphic function with rational coefficients $S^L(P) \in \mathcal{M}(V^*)$ so that the following properties hold:

1. *If P contains a line, then $S^L(P) = 0$.*
2. $$S^L(P)(\xi) = \sum_{y \in \Lambda_{V/L}} \int_{P \cap (y+L)} e^{\langle \xi, x \rangle}\, dm_L(x),$$ *for every $\xi \in V^*$ such that the above sum converges.*
3. *For every point $s \in \Lambda + L$, we have* $$S^L(s+P)(\xi) = e^{\langle \xi, s \rangle} S^L(P)(\xi).$$

Short formula for intermediate valuations

V. Baldoni, N. Berline, J. De Loera, **Kö.**, M. Vergne: Computation of the highest coefficients of weighted Ehrhart quasi-polynomials of rational polyhedra.
V. Baldoni, N. Berline, **Kö.**, M. Vergne: Intermediate Sums on Polyhedra: Computation and Real Ehrhart Theory.

Theorem (Short formula for $S^L(P)(\xi)$)

Fix a non-negative integer k_0. There exists a polynomial time algorithm for the following problem. Given the following input:

- (I_1) *a simple polytope $P \subset \mathbf{R}^d$, represented by its vertices, rational vectors $s_1, \dots, s_{d+1} \in \mathbf{Q}^d$ in binary encoding,*
- (I_2) *a subspace $L \subseteq \mathbf{Q}^d$ of codimension k_0, represented by $d - k_0$ linearly independent vectors $b_1, \dots, b_{d-k_0} \in \mathbf{Q}^d$ in binary encoding,*

compute the rational data such that we have the following equality of meromorphic functions:

$$S^L(P)(\xi) = \sum_{n \in N} \alpha^{(n)} \left(e^{\langle \xi, s^{(n)} \rangle} \prod_{i=1}^{k_0} T(z_i^{(n)}, \langle \xi, w_i^{(n)} \rangle) \right) \frac{1}{\prod_{i=1}^{d} \langle \xi, w_i^{(n)} \rangle}.$$

From this, we can extract intermediate sums of powers of linear forms $g(x) = \langle \ell, x \rangle^M$ using series expansions in $O(1)$ variables.
Sums of powers of linear forms generalize separable polynomial functions.

Powers of linear forms are enough: The polynomial Waring problem

J. Alexander and A. Hirschowitz, J. Algebraic Geom. **4** (1995), 201–222.

Theorem (Alexander–Hirschowitz, 1995)

A generic homogeneous polynomial of degree M in n variables is expressible as the sum of

$$r(M,n) = \left\lceil \frac{\binom{n+M-1}{M}}{n} \right\rceil$$

M-th powers of linear forms, with the exception of the cases $r(3,5)=8$, $r(4,3)=6$, $r(4,4)=10$, $r(4,5)=15$, and $M=2$, where $r(2,n)=n$. (Non-constructive.)

Theorem (Carlini–Catalisano–Geramita, 2011)

Minimal, constructive solution for monomials $\mathbf{x}^{\mathbf{M}}$, $M_1 \le \cdots \le M_n$ with $\prod_{i=2}^n (M_i+1)$, involving roots of unity.

Effective (constructive) version?

First numerical procedure given by J. Brachat, P. Comon, B. Mourrain, E. Tsigaridas (Lin. Alg. Appl., 2010)

Simple (suboptimal) rational constructions

$$\mathbf{x}^{\mathbf{M}} = \frac{1}{|\mathbf{M}|!} \sum_{0 \le p_i \le M_i} \alpha_{\mathbf{p}} (p_1 x_1 + \cdots + p_n x_n)^{|\mathbf{M}|}$$

with $\alpha_p = (-1)^{|\mathbf{M}|-(p_1+\cdots+p_n)} \binom{M_1}{p_1} \cdots \binom{M_n}{p_n}$

Three sources of computational difficulty

1. Size of the decomposition into powers of linear forms (especially for $g = f^p$ with large p)
   - Precompute the decomposition of $g(x) = (f(x) + s)^p$ as a function of the shift s
   - Numerical linear algebra techniques to compute decompositions.
   - Approximative decompositions into powers of linear forms?
   - Use different functions $g(x) = h(f(x))$?
   - For separable functions f over boxes, all cross terms can be removed.
   - Results for near-separable objective functions?
2. Arithmetic complexity (determinants) of vertex cones
   - Number of integer variables will have to be small enough.
   - Use discretization-free intermediate summation.
   - Relax integrality in some discrete directions.
3. Number of vertex cones
   - Assume number of constraints = dimension + $O(1)$.
   - Use "restriction formulations" with a penalty method (next slide)?

Size of restriction formulations and complexity of penalty methods

with Ph.D. student Yuan Zhou, forthcoming

Yannakakis' theorem:

- Let $P \subseteq \mathbf{R}^d$ be a polytope of dimension ≥ 1.
- Consider extended formulations $Q \subseteq \mathbf{R}^d \times \mathbf{R}^m$, i.e., $\{\, x \in \mathbf{R}^d : \exists y : (x, y) \in Q \,\} = P$.
- The extension complexity (smallest number of facets of any extended formulation) is equal to the non-negative rank of any slack matrix of P.
- Q can be made bounded at the cost of 1 extra facet.

Dualize:

- Consider "restriction formulations" $R \subseteq \mathbf{R}^d \times \mathbf{R}^m$, i.e., $\{\, x \in \mathbf{R}^d : (x, 0) \in R \,\} = P$.
- The "restriction–vertex-count complexity" (smallest number of vertices and rays of any restriction formulation) is equal to the non-negative rank of any slack matrix of P.
- R can be made bounded at the cost of 1 extra vertex.

Enter penalty methods:

$$\begin{array}{ll} \max & f(x) \\ \text{s.t.} & x \in P \end{array} \quad \longrightarrow \quad \begin{array}{ll} \max & f(x) \\ \text{s.t.} & (x, z) \in R \\ & z = 0 \end{array} \quad \longrightarrow \quad \begin{array}{ll} \max & f(x) - \sum_i h_i(z_i) \\ \text{s.t.} & (x, z) \in R \end{array}$$

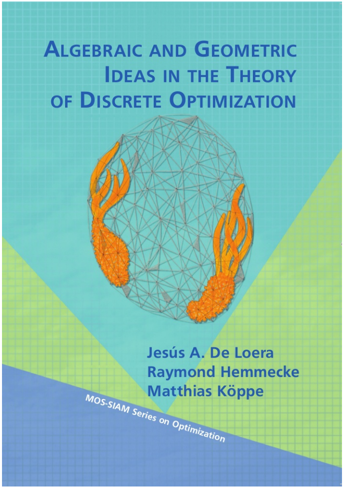
LattE integrale available at http://www.math.ucdavis.edu/~latte/

V. Baldoni, N. Berline, J. A. De Loera, M. Köppe, and M. Vergne.
Computation of the highest coefficients of weighted Ehrhart quasi-polynomials of rational polyhedra.
Foundations of Computational Mathematics, 12:435–469, 2012.

V. Baldoni, N. Berline, J. A. De Loera, M. Köppe, and M. Vergne.
Intermediate sums on polyhedra II: Bidegree and Poisson summation formula.
eprint arXiv:1404.0065 [math.CO], 2014.

V. Baldoni, N. Berline, M. Köppe, and M. Vergne.
Intermediate sums on polyhedra: Computation and real Ehrhart theory.
Mathematika, 59(1):1–22, September 2013.

J. A. De Loera, B. E. Dutra, M. Köppe, S. Moreinis, G. Pinto, and J. Wu.
Software for exact integration of polynomials over polyhedra.
Computational Geometry: Theory and Applications, 46(3):232–252, 2013.



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