Notes on volume approximation using SDP relaxations

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March 2023

Introduction. These notes are a crash course on how to approximate the volume of a compact semialgebraic set using semidefinite programming. What follows is entirely based on [HLS09, TWLH22, TLH23], but we implement the algorithms in `Mathematica`.

Our setting is the following. Let $K = \{x \in B \mid f(x) \geq 0\} \subset B \subset \mathbb{R}^n$ with $f = \sum_{w \in W} c_w x^w$ for some set W of multiindices. Here B is a nice set, by which we mean that the *moments* of B are known or easy to compute. For instance, in our examples, we are going to use the cube $B = [-1,1]^n$, but also the unit ball of any L_p-norm would do the job. Given a compact set $S \subset \mathbb{R}^n$ and a multiindex $\alpha \in \mathbb{Z}^n_{\geq 0}$, the α-th moment of S is

$$m_\alpha = \int_S x^\alpha \mathrm{d}\mu_S^*, \tag{1}$$

where μ_S^* is the Lebesgue measure on S. Note that $m_{\mathbf{0}} = \operatorname{vol} S$. The same definition works when we substitute μ_S^* with any other measure μ_S supported on S; in this case, we say that $\mathbf{m} = (m_\alpha)_\alpha$ has a representing finite Borel measure μ_S supported on S. In this way, we associate to the set S and the measure μ_S an infinite sequence of real numbers.

A few facts on moments. A natural question to ask is then: given a sequence of real numbers $\mathbf{m} = (m_\alpha)_\alpha$, does there exist a set S and a measure μ_S supported on S such that (1) holds?

Given $d \in \mathbb{N}$, denote by $\mathbb{N}^n_d$ the set of multiindices $\alpha \in \mathbb{Z}^n_{\geq 0}$ such that $|\alpha| = \alpha_1 + \ldots + \alpha_n \leq d$. Fix a set K as above, let $r = \lceil \frac{\deg f}{2} \rceil$, and consider a sequence of real numbers $\mathbf{m} = (m_\alpha)_\alpha$. Define the associated *moment matrix* and the *localizing matrix* to be respectively

$$M_d(\mathbf{m}) = \Big(m_{\alpha+\beta} \Big)_{\alpha,\beta \in \mathbb{N}^n_d}, \qquad M_{d-r}(f\mathbf{m}) = \Big(\sum_{w \in W} c_w m_{w+\alpha+\beta} \Big)_{\alpha,\beta \in \mathbb{N}^n_d}. \tag{2}$$

Notice that the moment matrix has size $\binom{n+d}{d} \times \binom{n+d}{d}$ whereas the localizing matrix has size $\binom{n+d-r}{d-r} \times \binom{n+d-r}{d-r}$. A necessary condition for a sequence $\mathbf{m} = (m_\alpha)_\alpha$ to have a representing measure supported on K is that for every $d \in \mathbb{N}$ the matrix inequalities

$M_d(\mathbf{m}) \succcurlyeq 0$ and $M_{d-r}(f\mathbf{m}) \succcurlyeq 0$ hold. This result is a formulation of Putinar's Positivstellensatz [Put93], also stated in [HLS09, Theorem 2.2]. In particular, the positive definiteness of the moment matrix is a necessary condition for $\mathbf{m}$ to have a representing measure; the inequality with the localizing matrix forces the support of the representing measure to be contained in the superlevel set $\{f(x) \geq 0\}$, namely K.

Example 1. As a sanity check, consider the disc $K = \{(x, y) \in \mathbb{R}^2 \mid f = 1 - x^2 - y^2 \geq 0\}$. One can compute its moments via the formula

$$m_{(\alpha_1,\alpha_2)} = ((-1)^{\alpha_1} + 1)\,((-1)^{\alpha_2} + 1)\,\frac{\Gamma\left(\frac{\alpha_1+1}{2}\right)\Gamma\left(\frac{\alpha_2+1}{2}\right)}{4\Gamma\left(\frac{1}{2}(\alpha_1 + \alpha_2 + 4)\right)}.$$

For $d = 3$, the moment and localizing matrices in (2) are

$$M_3(\mathbf{m}) = \begin{pmatrix} \pi & 0 & \frac{\pi}{4} & 0 & 0 & 0 & 0 & \frac{\pi}{4} & 0 & 0 \\ 0 & \frac{\pi}{4} & 0 & \frac{\pi}{8} & 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 \\ \frac{\pi}{4} & 0 & \frac{\pi}{8} & 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 & 0 \\ 0 & \frac{\pi}{8} & 0 & \frac{5\pi}{64} & 0 & 0 & 0 & 0 & \frac{\pi}{64} & 0 \\ 0 & 0 & 0 & 0 & \frac{\pi}{4} & 0 & \frac{\pi}{24} & 0 & 0 & \frac{\pi}{8} \\ 0 & 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\pi}{24} & 0 & \frac{\pi}{64} & 0 & 0 & \frac{\pi}{64} \\ \frac{\pi}{4} & 0 & \frac{\pi}{24} & 0 & 0 & 0 & 0 & \frac{\pi}{8} & 0 & 0 \\ 0 & \frac{\pi}{24} & 0 & \frac{\pi}{64} & 0 & 0 & 0 & 0 & \frac{\pi}{64} & 0 \\ 0 & 0 & 0 & 0 & \frac{\pi}{8} & 0 & \frac{\pi}{64} & 0 & 0 & \frac{5\pi}{64} \end{pmatrix}, \quad M_2(f\mathbf{m}) = \begin{pmatrix} \frac{\pi}{2} & 0 & \frac{\pi}{12} & 0 & 0 & \frac{\pi}{12} \\ 0 & \frac{\pi}{12} & 0 & 0 & 0 & 0 \\ \frac{\pi}{12} & 0 & \frac{\pi}{32} & 0 & 0 & \frac{\pi}{96} \\ 0 & 0 & 0 & \frac{\pi}{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\pi}{96} & 0 \\ \frac{\pi}{12} & 0 & \frac{\pi}{96} & 0 & 0 & \frac{\pi}{32} \end{pmatrix},$$

which are indeed positive definite.

Infinite-dimensional LP and its dual. In this section we construct an infinite-dimensional *Linear Program* on measures whose optimal value is the volume of $K \subset B$. The program is stated in [HLS09, Equation 3.1], [TWLH22, Equation 1], and it reads:

$$\begin{aligned} P: \qquad & \max_{\mu_K, \mu_{B\setminus K}} \int \mathrm{d}\mu_K \\ & \text{s.t.} \quad \mu_K + \mu_{B\setminus K} = \mu_B^*, \end{aligned} \tag{3}$$

where μ_S is a positive finite Borel measure supported on S, and μ_B^* is the Lebesgue measure on B. The adjective "infinite-dimensional" refers to the fact that we are optimizing over a set of measures, which is uncountable. Based on the theory of dual Banach spaces, one can talk about dual convex bodies or convex cones, and construct the theory of dual programming. In our case, it is a well-known fact (from some analysis class) that the dual to the space of positive finite Borel measures is the set of positive continuous functions. This observation leads to the definition of an LP dual to P:

$$\begin{aligned} P^*: \qquad & \inf_{\gamma} \int \gamma \, \mathrm{d}\mu_B^* \\ & \text{s.t.} \quad \gamma \geq \mathbb{1}_K, \end{aligned} \tag{4}$$

where γ is a positive continuous function on B and $\mathbb{1}_K$ is the indicator function of K. It can be proved that there is no duality gap between P and P^*, which means that the optimal values of (3) and (4) coincide. Notice that the optimal value of P^* is an infimum and not a minimum, since we are trying to approximate the *discontinuous* indicator function $\mathbb{1}_K$ using continuous functions. This detail will turn out to be relevant for the slow rate of approximation that this method has in the first place.

Finite-dimensional SDP and its dual. The infinite-dimensional LP can be approximated as closely as desired by using a hierarchy of finite-dimensional *SemiDefinite Programs*, see [Las10]. The sequence of optimal values of the hierarchy converges monotonically to the optimal value of the LP [HLS09, Theorem 3.2]. There is again a primal and dual version of the SDP problems. In our setting, the primal hierarchy is

$$\begin{aligned} P_d: \qquad & \max_{\mathbf{m},\widehat{\mathbf{m}}} \ m_{\mathbf{0}} \\ & \text{s.t.} \ \ \mathbf{m}+\widehat{\mathbf{m}}=\mathbf{b}, \\ & \qquad M_d(\mathbf{m}) \succcurlyeq 0,\ M_d(\widehat{\mathbf{m}}) \succcurlyeq 0, \\ & \qquad M_{d-r}(f\mathbf{m}) \succcurlyeq 0, \end{aligned} \tag{5}$$

where $\mathbf{m} = (m_\alpha)_{\alpha\in\mathbb{N}^n_{2d}}$, $\widehat{\mathbf{m}} = (\widehat{m}_\alpha)_{\alpha\in\mathbb{N}^n_{2d}}$, and $\mathbf{b}$ is the sequence of moments of B for the multiindices in $\mathbb{N}^n_{2d}$. This formulation is [TWLH22, Equation 3] but also [HLS09, Equation 3.3]. Note that the optimal value of P_d is an upper bound for $\operatorname{vol}(K)$, since we are optimizing over a larger set. The corresponding dual SDP is [HLS09, Equation 3.6], which is formulated using sums of squares of polynomials. The authors of [HLS09, TWLH22, TLH23] implemented the SDPs using `GloptiPoly MATLAB` [HLL09]. Our basic computations in the next examples are performed in `Mathematica`. We are going to include the linear condition $\mathbf{m}+\widehat{\mathbf{m}}=\mathbf{b}$ inside the condition on the moment matrix of $\widehat{\mathbf{m}}$, by imposing directly that $M_d(\mathbf{b}-\mathbf{m}) \succcurlyeq 0$.

Example 2 (The TV screen in Figure 1, left)**.** Consider the semialgebraic convex body $K_1 = \{x, y \in [-1.2, 1.2]^2 \mid f_1(x, y) \geq 0\} \subset \mathbb{R}^2$ with

$$f_1(x,y) = 1 - x^4 - y^4 - \frac{1}{100}xy.$$

Using for instance the methods from [LMSED19] we can compute the volume of K_1, namely 3.7081599447.... Let us now use the SDP formulation. Fix $d = 10$, then $M_{10}(\mathbf{m})$ and $M_{10}(\mathbf{b}-\mathbf{m})$ are 66×66 matrices, and for instance the second one is

$$\begin{pmatrix} 4-m_{(0,0)} & -m_{(0,1)} & \frac{4}{3}-m_{(0,2)} & -m_{(0,3)} & \cdots \\ -m_{(0,1)} & \frac{4}{3}-m_{(0,2)} & -m_{(0,3)} & \frac{4}{5}-m_{(0,4)} & \cdots \\ \frac{4}{3}-m_{(0,2)} & -m_{(0,3)} & \frac{4}{5}-m_{(0,4)} & -m_{(0,5)} & \cdots \\ -m_{(0,3)} & \frac{4}{5}-m_{(0,4)} & -m_{(0,5)} & \frac{4}{7}-m_{(0,6)} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

The matrix $M_8(f_1\mathbf{m})$ is a 45×45 matrix whose (α,β) entry is

$$m_{\alpha+\beta} - m_{(4,0)+\alpha+\beta} - m_{(0,4)+\alpha+\beta} - \frac{1}{100}m_{(1,1)+\alpha+\beta}.$$

The optimal value of the semidefinite program P_{10} is 4.4644647361..., the optimal value of P_{14} is 4.3679560947..., and for P_{18} we get 4.3241824171...; these numbers provide upper bounds for the actual volume, as predicted.

Example 3 (The elliptope in Figure 1, right)**.** Consider the semialgebraic convex body $K_2 = \{x, y \in [-1, 1]^3 \mid f_2(x, y) \geq 0\} \subset \mathbb{R}^3$ with

$$f_2(x,y) = 1 - x^2 - y^2 - z^2 + 2xyz.$$

The volume of this spectrahedron, called elliptope, can be computed analytically and it is $\operatorname{vol} K_2 = \frac{\pi^2}{2} = 4.934802202....$ In this case the solutions of the SDP for $d = 4, 8, 12$ are respectively 7.3254012963..., 6.6182632506..., and 6.303035372....

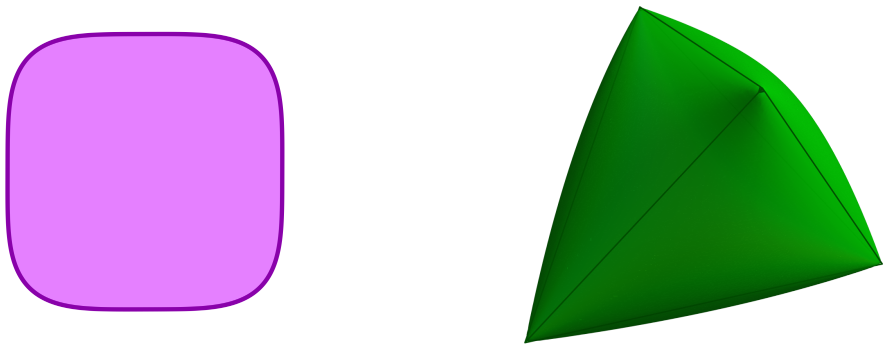


Figure 1: Left: the TV screen from Example 2. Right: the elliptope from Example 3.

Stokes constraints. As the reader can notice in Example 2 and Example 3, the convergence of the approximation via the SDP method is quite slow. Indeed, in [KH18] the authors prove that, under mild assumptions, the convergence rate is $\mathcal{O}(\frac{1}{\log\log d})$. The goal of this section is to improve the convergence by using *Stokes constraints*, introduced and analysed in [Las17, TWLH22, TLH23].

As we already pointed out, in the infinite-dimensional linear program P^* (and in its corresponding SDP hierarchy) we want to approximate a piecewise-differentiable function, $\mathbb{1}_K$, with continuous functions (respectively, polynomials). This produces the well-known *Gibbs effect*, creating many oscillations near the boundary of K in the polynomial solutions of the SDP.

Heuristically, one could try to speed up the computation by adding certain linear constraint that do not modify the infinite-dimensional LP problem but add more information to the finite-dimensional SDP. One concrete way to do this uses Stokes' theorem (and its consequences) and the fact that f vanishes on the boundary of K.

Let U be an open set such that the Euclidean closure of U is our set K. Since ∂K is smooth almost everywhere, the classical Stokes' theorem applies, namely

$$\int_{\partial K} \omega = \int_K \mathrm{d}\omega$$

for any $(n-1)$-differential form ω on $\mathbb{R}^n$. One of the consequences of this theorem is the following integral inequality, known as the Gauss formula:

$$\int_{\partial K} V(x) \cdot \widehat{n}(x) \; \mathrm{d}\mathcal{H}^{n-1}(x) = \int_K \operatorname{div} V(x) \; \mathrm{d}x,$$

where $V(x)$ is a vector field, $\widehat{n}(x)$ is the exterior normal vector at $x \in \partial K$, $\mathcal{H}^{n-1}$ is the $(n-1)$-dimensional Hausdorff measure, and div denotes the divergence. If the vector field is just a scalar field multiplying a constant vector, namely $V(x) = v(x)c$, then we obtain the following chain of equalities:

$$c \cdot \left(\int_{\partial K} v(x)\widehat{n}(x) \; \mathrm{d}\mathcal{H}^{n-1}(x) \right) = \int_K \operatorname{div} \big(v(x)c \big) \; \mathrm{d}x = c \cdot \left(\int_K \nabla v(x) \; \mathrm{d}x \right)$$

because $\operatorname{div} \big(v(x)c \big) = \nabla v(x) \cdot c + v(x) \operatorname{div} c$ and the divergence of a constant vector is zero. Since this equality must be valid for every $c \in \mathbb{R}^n$, we have

$$\int_{\partial K} v(x)\widehat{n}(x) \; \mathrm{d}\mathcal{H}^{n-1}(x) = \int_K \nabla v(x) \; \mathrm{d}x. \tag{6}$$

If $v = 0$ on ∂K, then the left hand side of (6) is zero. This condition can be expressed in terms of measures and distributions, and added to (3) and (4) as in [TWLH22, Equation 17 and Remark 3]. In the more concrete case of the SDP, the Stokes constraints translate as follows. Let $v(x) = f(x)x^\alpha$ for any multiindex $\alpha \in \mathbb{N}^n$ with $|\alpha| \leq d + 1 - \deg f$. Then we require that

$$\nabla\Big(f(x)x^\alpha\Big)\Big|_{x^\beta \to m_\beta} = 0,$$

where we substitute each monomial with the corresponding moment, and get n new linear conditions for every such α.

Example 4. Consider the two convex bodies from Example 2 and Example 3. The Stokes constraints for a given α are:

$$\begin{aligned}
&K_1 : \\
&\alpha_1 m_{\alpha+(-1,0)} - (\alpha_1+4)m_{\alpha+(3,0)} - \alpha_1 m_{\alpha+(-1,4)} - \tfrac{\alpha_1+1}{100} m_{\alpha+(0,1)} = 0, \\
&\alpha_2 m_{\alpha+(0,-1)} - \alpha_2 m_{\alpha+(4,-1)} - (\alpha_2+4)m_{\alpha+(0,3)} - \tfrac{\alpha_2+1}{100} m_{\alpha+(1,0)} = 0, \\
&K_2 : \\
&\alpha_1 m_{\alpha+(-1,0,0)} - (\alpha_1+2)m_{\alpha+(1,0,0)} - \alpha_1 m_{\alpha+(-1,2,0)} - \alpha_1 m_{\alpha+(-1,0,2)} + 2(\alpha_1+1)m_{\alpha+(0,1,1)} = 0, \\
&\alpha_2 m_{\alpha+(0,-1,0)} - \alpha_2 m_{\alpha+(2,-1,0)} - (\alpha_2+2)m_{\alpha+(0,1,0)} - \alpha_2 m_{\alpha+(0,-1,2)} + 2(\alpha_2+1)m_{\alpha+(1,0,1)} = 0, \\
&\alpha_3 m_{\alpha+(0,0,-1)} - \alpha_3 m_{\alpha+(2,0,-1)} - \alpha_3 m_{\alpha+(0,2,-1)} - (\alpha_3+2)m_{\alpha+(0,0,1)} + 2(\alpha_3+1)m_{\alpha+(1,1,0)} = 0.
\end{aligned}$$

Table 1 compares the computation of the optimal value of the SDP (5) with and without Stokes constraints.

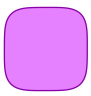
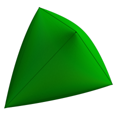
K	Volume	d	without Stokes		with Stokes	
			max P_d	time	max P_d	time
	3.708159...	10	4.464464...	0.621093	3.709994...	0.482376
		14	4.367956...	3.545369	3.708191...	3.738137
		18	4.324182...	14.906281	3.708163...	20.592531
	4.934802...	4	7.325401...	0.124392	5.612716...	0.077315
		8	6.618263...	7.222441	4.976796...	7.178571
		12	6.303035...	696.886298	4.937648...	1105.619231

Table 1: Comparison of the optimal values of (5), with and without Stokes constraints, in Example 2 and Example 3. The column "max P_d" displays the optimal value of P_d for a certain d, whereas the column "time" gives the time, in seconds, involved in running the command `SemidefiniteOptimization` in `Mathematica`.

Conclusions. As Table 1 shows, the convergence with Stokes constraints is much faster than without constraints. The heuristics is that now, with the (dual version of the) Stokes constraints added to P^*, the function we are trying to approximate is not just the indicator function of K. A more precise explanation can be found in [TLH23], for a slightly different type of Stokes constraints. The authors, in fact, prove that when adding this new type of constraints, obtained again from Stokes theorem, the optimal solution of the new P^* becomes a minimum. This eliminates any kind of Gibbs effect, and guarantees a faster convergence. In [TLH23], the authors mention that, from numerical experiments, it is reasonable to expect that the original Stokes constraints and the new Stokes constraints are equivalent, but there is no formal proof of this statement yet.

We conclude by mentioning that more general semialgebraic sets fit into the framework of [HLS09, TWLH22, TLH23], and we refer to these works for all the proofs, much more detailed computations and deeper analyses from a numerical point of view.

References

[HLL09] Didier Henrion, Jean-Bernard Lasserre, and Johan Löfberg. GloptiPoly 3: moments, optimization and semidefinite programming. *Optimization Methods & Software*, 24(4-5):761–779, 2009.

[HLS09] Didier Henrion, Jean Bernard Lasserre, and Carlo Savorgnan. Approximate volume and integration for basic semialgebraic sets. *SIAM Review*, 51(4):722–743, 2009.

[KH18] Milan Korda and Didier Henrion. Convergence rates of moment-sum-of-squares hierarchies for volume approximation of semialgebraic sets. *Optimization Letters*, 12(3):435–442, 2018.

[Las10] Jean Bernard Lasserre. *Moments, positive polynomials and their applications*, volume 1 of *Imperial College Press Optimization Series*. Imperial College Press, London, 2010.

[Las17] Jean B. Lasserre. Computing Gaussian & exponential measures of semi-algebraic sets. *Advances in Applied Mathematics*, 91:137–163, 2017.

[LMSED19] Pierre Lairez, Marc Mezzarobba, and Mohab Safey El Din. Computing the volume of compact semi-algebraic sets. In *Proceedings of the 2019 on International Symposium on Symbolic and Algebraic Computation*, page 259–266, New York, NY, USA, 2019. Association for Computing Machinery.

[Put93] Mihai Putinar. Positive polynomials on compact semi-algebraic sets. *Indiana University Mathematics Journal*, 42(3):969–984, 1993.

[TLH23] Matteo Tacchi, Jean Bernard Lasserre, and Didier Henrion. Stokes, Gibbs, and Volume Computation of Semi-Algebraic Sets. *Discrete & Computational Geometry. An International Journal of Mathematics and Computer Science*, 69(1):260–283, 2023.

[TWLH22] Matteo Tacchi, Tillmann Weisser, Jean Bernard Lasserre, and Didier Henrion. Exploiting sparsity for semi-algebraic set volume computation. *Foundations of Computational Mathematics. The Journal of the Society for the Foundations of Computational Mathematics*, 22(1):161–209, 2022.