Computing integral asymptotics using toric blow-ups of ideals

Shaowei Lin (UC Berkeley)

shaowei@math.berkeley.edu

23 Oct 2011, Salt Lake City

AMS Special Session on Computational and Algorithmic Algebraic Geometry

Laplace Integrals

Laplace integrals of the form

$$Z(N) = \int_W e^{-Nf(\omega)} \varphi(\omega) \, d\omega$$

occur frequently in machine learning, computational biology and combinatorics. Here, N is a positive real number, $W \subset \mathbb{R}^d$ is a small nbhd of the origin, and f and φ are real-valued analytic functions where f attains its minimum at the origin.

We are often interested in *approximating* $Z(N)$ for large N.

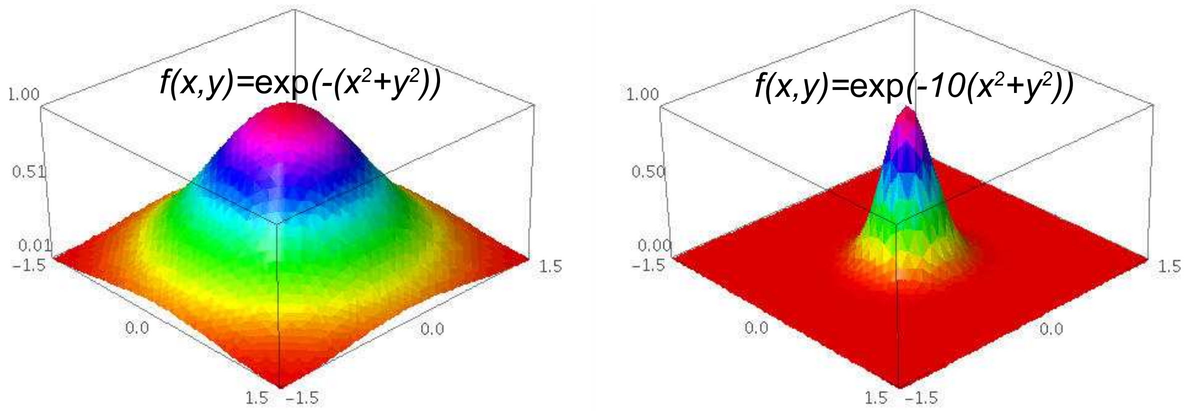
Example:
In *statistics*, $Z(N)$ may be a marginal likelihood integral used in model selection. We usually approximate such integrals using MCMC methods.
In *combinatorics*, $Z(N)$ may be the coefficient of a rational generating function, representing the count of an interesting combinatorial object.

Laplace Approximation

Example: Let $H(\omega)$ be the Hessian of f. If $H(0) \succ 0$ and $\varphi(0) > 0$, then asymptotically

$$Z(N) \;\approx\; e^{-Nf(0)} \cdot \varphi(0) \sqrt{\frac{(2\pi)^d}{\det H(0)}} \cdot N^{-d/2} \quad \text{as } N \to \infty.$$

Note that the integral asymptotics depend on the *geometry* of the function f near its minimum points.



Remark: This formula is used to prove Stirling's approximation.

Asymptotic Theory

More generally, even if $\det H(0) = 0$, Arnol'd–Guseĭn-Zade–Varchenko showed that asymptotically,

$$Z(N) \;\approx\; e^{-Nf(0)} \cdot CN^{-\lambda}(\log N)^{\theta-1}, \quad N \to \infty$$

for some positive $C \in \mathbb{R}$, $\lambda \in \mathbb{Q}$, $\theta \in \mathbb{Z}$. Here, λ is the *real log canonical threshold* of f, and θ its *multiplicity*. We denote $\mathrm{RLCT}(f;\varphi) := (\lambda, \theta)$.

Theorem (AGV):

> The RLCT λ of f is the smallest pole of the zeta function
>
> $$\zeta(z) = \int_W f(\omega)^{-z}\varphi(\omega)d\omega, \quad z \in \mathbb{C},$$
>
> and θ is the multiplicity of this pole.

The poles of $\zeta(z)$ are computed using a *resolution of singularities* of f.

Regularly Parametrized Functions

We were inspired by our statistical examples to study *regularly parametrized analytic* functions f, i.e. f is a composition of maps

$$W \xrightarrow{g} U \xrightarrow{h} \mathbb{R}$$

where $W \subset \mathbb{R}^d, U \subset \mathbb{R}^k$ are small nbhds of the origin 0, h attains its minimum uniquely at 0 and the Hessian of h is positive definite at 0.

We also assume that g is a *polynomial* map, and we want to exploit this polynomiality in our computations.

Goal of this talk:

- Show how to use *ideal-theoretic methods* to find a resolution of singularities for such functions f and to compute its RLCT.
- Compute the *leading coefficient* C in the asymptotics of $Z(N)$.

Ideal-theoretic Methods

Sos-nondegeneracy

Let $[\omega^\alpha]f$ denote the coefficient of a monomial ω^α in a polynomial f.
Recall that f is singular at $x \in \mathbb{R}^d$ if $f(x) = 0$ and $\nabla f(x) = 0$.

Definitions (Varchenko): Let $f \in \mathbb{R}[\omega]$ be a polynomial.
Newton polyhedron $\mathcal{P}(f) = \operatorname{conv}\{\alpha \in \mathbb{R}^d : [\omega^\alpha]f \neq 0\}$.
Given $\gamma \subset \mathbb{R}^d$, *face polynomial* $f_\gamma = \sum_{\alpha \in \gamma}([\omega^\alpha]f)\omega^\alpha$.
We say f is *nondegenerate* if f_γ is nonsingular at all $x \in (\mathbb{R}^*)^d$ for all compact faces $\gamma \in \mathcal{P}(f)$.

Definitions (L.): Let $I \subset \mathbb{R}[\omega]$ be an ideal.
Newton polyhedron $\mathcal{P}(I) = \operatorname{conv}\{\alpha \in \mathbb{R}^d : [\omega^\alpha]f \neq 0$ for some $f \in I\}$.
Given $\gamma \subset \mathbb{R}^d$, *face ideal* $I_\gamma = \langle f_\gamma : f \in I \rangle$.
We say I is *sos-nondegenerate* if $f_1^2 + \ldots + f_r^2$ is nondegenerate for some generating set $\{f_1, \ldots, f_r\}$.

Remark: sos = sum-of-squares.

Sos-nondegeneracy

Proposition (L.):
If $I = \langle f_1, \ldots, f_r \rangle$ and $\gamma \subset \mathcal{P}(I)$ is a compact face, then $I_\gamma = \langle f_{1\gamma}, \ldots, f_{r\gamma} \rangle$.

We have the following *equivalent definitions* of sos-nondegeneracy.

Proposition (L.):

1. For some generating set $\{f_1, \ldots, f_r\}$, $f_1^2 + \ldots + f_r^2$ is nondegenerate.
2. For all generating sets $\{f_1, \ldots, f_r\}$, $f_1^2 + \ldots + f_r^2$ is nondegenerate.
3. For all compact faces $\gamma \subset \mathcal{P}(I)$, the real variety $\mathcal{V}(I_\gamma)$ does not intersect the torus $(\mathbb{R}^*)^d$.

Remark: We discovered later that Saia has a notion of nondegeneracy similar to (3) for ideals in the ring of *complex* formal power series.

Proposition (Zwiernik):
Monomial ideals are sos-nondegenerate.

Fiber Ideals

Let $f : W \xrightarrow{g} U \xrightarrow{h} \mathbb{R}, W \subset \mathbb{R}^d, U \subset \mathbb{R}^k$ be regularly parametrized. Suppose $g(0) = 0$, $h(0) = 0$, and the minimum of h is attained at 0. Define the *fiber ideal* $\langle g_1(\omega), \ldots, g_k(\omega) \rangle$. It is the ideal of the fiber $g^{-1}(0)$.

Define $\mathrm{RLCT}(I; \varphi)$ of an ideal $I = \langle g_1, \ldots, g_k \rangle$ to be the smallest pole and its multiplicity of the zeta function

$$\zeta(z) = \int_W (g_1^2 + \cdots + g_k^2)^{-z/2} \varphi(\omega) d\omega.$$

Proposition (L):
$\mathrm{RLCT}(f; \varphi) = (\lambda/2, \theta)$, where $(\lambda, \theta) = \mathrm{RLCT}(I; \varphi)$.

Proposition (L.):
Let $\rho : \mathcal{M} \to W$ be a principalization map for the fiber ideal I, i.e. the pullback $\rho^{-1}(I)$ is locally principal on $\mathcal{M}$. Then, ρ desingularizes f.

Toric Blowups

Let $\mathcal{F}$ be a *smooth polyhedral fan* supported on the positive orthant $\mathbb{R}^d_{\geq 0}$.
[smooth: each cone is generated by a subset of some basis of $\mathbb{Z}^d$]

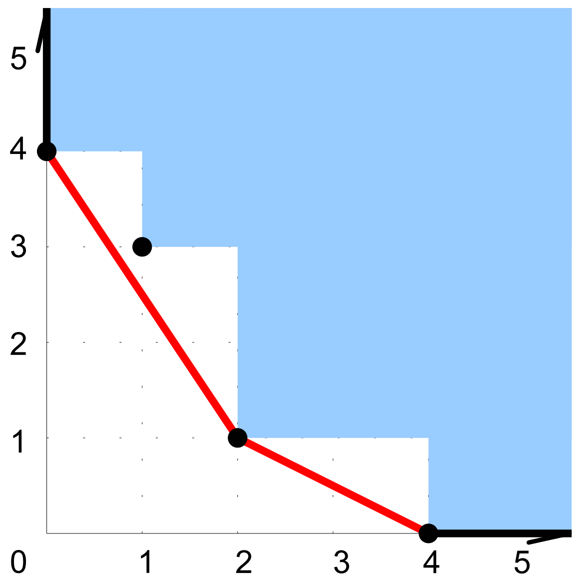
Recall that we can associate to $\mathcal{F}$, a *toric variety* $\mathbb{P}(\mathcal{F})$ covered by open affines $U_\sigma \simeq \mathbb{R}^d$, one for each maximal cone σ of $\mathcal{F}$.

We also have a *blowup map* $\rho_{\mathcal{F}} : \mathbb{P}(\mathcal{F}) \to \mathbb{R}^d$ described by monomial maps $\rho_{\mathcal{F},\sigma} : U_\sigma \to \mathbb{R}^d, \mu \mapsto \mu^\nu$, on the open affines.
[The columns of the matrix ν are minimal generators of the maximal cone σ, and $(\mu^\nu)_i = \mu^{\nu_i}$ where ν_i is the ith row of ν.]

Proposition (L.):
Given a fiber ideal I, let $\mathcal{F}$ be a *smooth refinement* of the normal fan of the Newton polyhedron $\mathcal{P}(I)$. If I is sos-nondegenerate, then the toric blowup $\rho_{\mathcal{F}} : \mathbb{P}(\mathcal{F}) \to \mathbb{R}^d$ desingularizes f.

Asymptotic Lower Bound

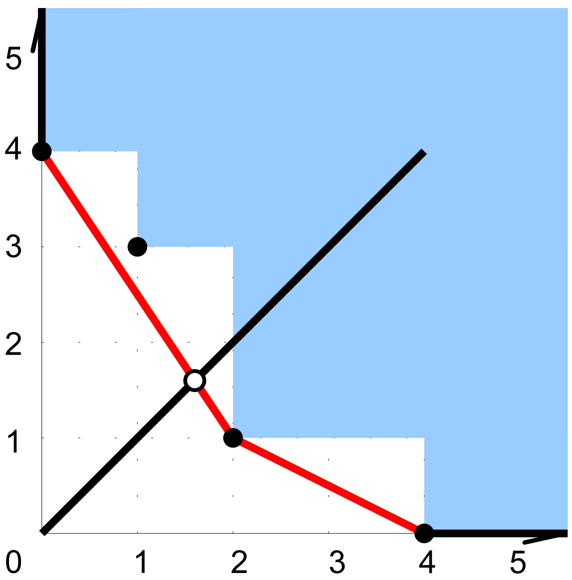
Given $\tau \in \mathbb{Z}^d_{\geq 0}$, define the *$\tau$-distance* l_τ of a polyhedron $\mathcal{P} \subset \mathbb{R}^d$ to be the smallest $t \geq 0$ such that $t(\tau_1 + 1, \ldots, \tau_d + 1) \in \mathcal{P}$, and its *multiplicity* θ_τ to be the codim of the face of $\mathcal{P}$ at this intersection.



Let $I = \langle x^4, x^2y, xy^3, y^4 \rangle$.

Asymptotic Lower Bound

Given $\tau \in \mathbb{Z}^d_{\geq 0}$, define the *$\tau$-distance* l_τ of a polyhedron $\mathcal{P} \subset \mathbb{R}^d$ to be the smallest $t \geq 0$ such that $t(\tau_1 + 1, \ldots, \tau_d + 1) \in \mathcal{P}$, and its *multiplicity* θ_τ to be the codim of the face of $\mathcal{P}$ at this intersection.

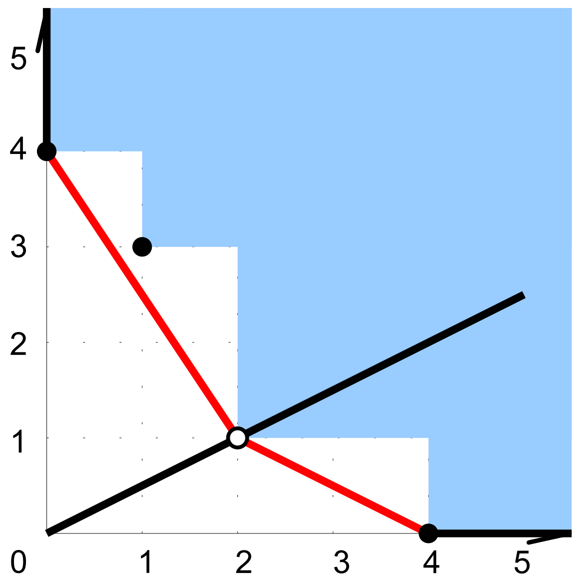


Let $I = \langle x^4, x^2y, xy^3, y^4 \rangle$.

For $\tau = (0,0)$: $\quad l_\tau = 8/5$, $\theta_\tau = 1$.

Asymptotic Lower Bound

Given $\tau \in \mathbb{Z}^d_{\geq 0}$, define the *$\tau$-distance* l_τ of a polyhedron $\mathcal{P} \subset \mathbb{R}^d$ to be the smallest $t \geq 0$ such that $t(\tau_1 + 1, \ldots, \tau_d + 1) \in \mathcal{P}$, and its *multiplicity* θ_τ to be the codim of the face of $\mathcal{P}$ at this intersection.



Let $I = \langle x^4, x^2y, xy^3, y^4 \rangle$.

For $\tau = (0,0) : \quad l_\tau = 8/5$, $\theta_\tau = 1$.

For $\tau = (1,0) : \quad l_\tau = 1$, $\theta_\tau = 2$.

Asymptotic Lower Bound

Given $\tau \in \mathbb{Z}^d_{\geq 0}$, define the *$\tau$-distance* l_τ of a polyhedron $\mathcal{P} \subset \mathbb{R}^d$ to be the smallest $t \geq 0$ such that $t(\tau_1 + 1, \ldots, \tau_d + 1) \in \mathcal{P}$, and its *multiplicity* θ_τ to be the codim of the face of $\mathcal{P}$ at this intersection.

Theorem (L.):
Given a regularly parametrized function f and a vector $\tau \in \mathbb{Z}^d_{\geq 0}$, let I be the fiber ideal and let (l_τ, θ_τ) be the t-distance and its multiplicity of the Newton polyhedron $\mathcal{P}(I)$. Then, asymptotically

$$Z(N) = \int_W e^{-Nf(\omega)} \omega^\tau d\omega$$

is *bounded below* by $CN^{-1/(2l_\tau)}(\log N)^{\theta_\tau - 1}$ for some constant C.
This bound is tight if the fiber ideal I is sos-nondegenerate.

In other words, if I is sos-ndg, then $\mathrm{RLCT}(I; \omega^\tau) = (1/l_\tau, \theta_\tau)$.
[This is the *real analog* of Howard's result for complex LCTs.]

Leading Coefficients

Preliminaries

We want to compute the leading coefficient C in the asymptotics

$$Z(N) = \int_{[0,\varepsilon]^d} e^{-Nf(\omega)} \omega^\tau d\omega \;\approx\; CN^{-\lambda}(\log N)^{\theta-1}.$$

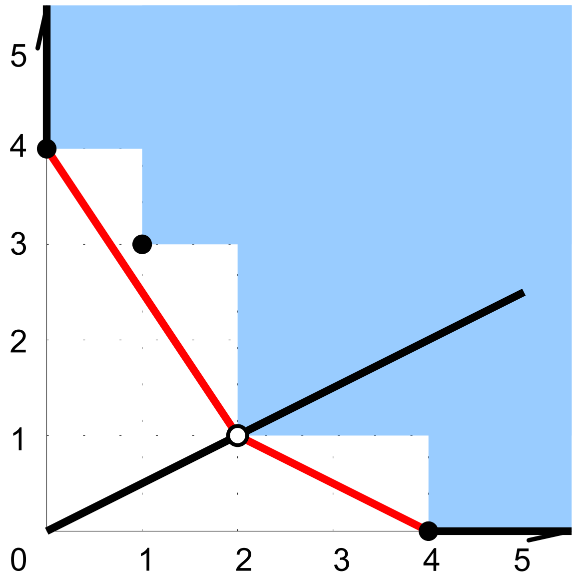
where f is *nondegenerate*, ε is *sufficiently small* and $\tau \in \mathbb{Z}^d_{\geq 0}$.

Because f is nondegenerate, any smooth refinement of the normal fan of the Newton polyhedron $\mathcal{P}(f)$ desingularizes f at the origin. We fix $\mathcal{F}$ to be one such refinement.

We pick ε to be sufficiently small so that under the blowup $\rho_\mathcal{F}$, the strict transform g of f is positive at every point in $\rho_\mathcal{F}^{-1}[0,\varepsilon]^d$.

By scaling the coordinates ω, we may assume for simplicity that $\varepsilon = 1$.

Preliminaries



Recall that $(\lambda, \theta) = (1/l_\tau, \theta_\tau)$ where l_τ is the τ-distance of the Newton polyhedron $\mathcal{P}(f)$ and θ_τ its multiplicity.

Let σ_τ be the cone in the normal fan of $\mathcal{P}(f)$ corresponding to the face at this intersection. Note that σ_τ has dimension θ.

In the refinement $\mathcal{F}$, we consider the set $\mathcal{F}_\tau$ of all maximal cones which intersect σ_τ in dimension θ. For each σ in $\mathcal{F}_\tau$, let ν be the matrix whose columns are the minimal generators of σ and where the first θ columns are generators of σ_τ.

Leading Coefficient

Theorem (L.):
The leading coefficient C in the asymptotics of $Z(N)$ equals

$$\frac{\Gamma(\lambda)}{(\theta-1)!}\sum_{\sigma\in\mathcal{F}_\tau}\prod_{i=1}^{\theta}(\nu\alpha)_i^{-1}\int_{[0,1]^{d-\theta}} g(0,\bar{\mu})^{-\lambda}\bar{\mu}^{\overline{m}-1}d\bar{\mu}.$$

Here, $\Gamma(\cdot)$ is the Gamma function, and for each σ in $\mathcal{F}_\tau$,

ν is the matrix of minimal generators,

$\alpha\in\mathcal{P}(f)$ is the vertex dual to σ,

$\mu=(\hat{\mu},\bar{\mu})\in\mathbb{R}^\theta\times\mathbb{R}^{d-\theta}$,

$m=\nu(-\lambda\alpha+\tau+1)=(\hat{m},\overline{m})\in\mathbb{R}^\theta\times\mathbb{R}^{d-\theta}$, and

$g(\hat{\mu},\overline{\mu})=f(\mu^\nu)\mu^{-\nu\alpha}$ is the strict transform of f in the open affine U_σ.

Work in Progress: `Macaulay2` code which implements this formula.

Example

Question: Find the first term asymptotics of the integral

$$Z(N) = \int_{[0,1]^2} (1 - x^2y^2)^{N/2}\, dxdy.$$

[This question comes from a statistical example involving coin tosses.]

Solution: Rewrite the integral as $Z(N) = \int_{[0,1]^2} e^{-Nf(x,y)} dxdy$ where

$$f(x,y) = -\frac{1}{2}\log(1 - x^2y^2).$$

Here, f is regularly parametrized, because it is the composition of maps $(x,y) \mapsto xy$ and $t \mapsto -\frac{1}{2}\log(1-t^2)$. The fiber ideal $I = \langle xy \rangle$ is monomial and sos-nondegenerate. Thus, f is nondegenerate and the Newton polyhedron $\mathcal{P}(f)$ is the orthant cornered at $(2,2)$. Using our formula, we get

$$Z(N) \;\approx\; \sqrt{\frac{\pi}{8}}\, N^{-1/2} \log N.$$

Example

In fact, using similar techniques, we get the asymptotic expansion $Z(N) \approx \sum_{\lambda,\theta} C_{\lambda,\theta} N^{-\lambda} (\log N)^{\theta-1}$ where the first few terms are

$$C_{\frac{1}{2},2} = \sqrt{\frac{\pi}{8}}, \qquad C_{\frac{1}{2},1} = -\sqrt{\frac{\pi}{8}} \left(\frac{1}{\log 2} - 2\log 2 - \gamma \right),$$

$$C_{1,2} = -\frac{1}{4}, \qquad C_{1,1} = \frac{1}{4} \left(\frac{1}{\log 2} + 1 - \gamma \right),$$

$$C_{\frac{3}{2},2} = -\frac{\sqrt{2\pi}}{128}, \qquad C_{\frac{3}{2},1} = \frac{\sqrt{2\pi}}{128} \left(\frac{1}{\log 2} - 2\log 2 - \frac{10}{3} - \gamma \right),$$

$$C_{2,2} = 0, \qquad C_{2,1} = -\frac{1}{24}.$$

Here, γ is the Euler-Macheroni constant

$$\gamma = \lim_{n\to\infty} \left(\sum_{i=1}^{n} \frac{1}{k} - \log n \right) \approx 0.5772156649.$$

“Algebraic Methods for Evaluating Integrals in Bayesian Statistics”

http://math.berkeley.edu/~shaowei/swthesis.pdf

(PhD dissertation, May 2011)

References

1. D. Cox, J. Little and H. Schenck: *Toric Varieties*. Amer. Math. Soc., 2011.
2. D. Cox, J. Little and D. O'Shea: *Ideals, Varieties, and Algorithms: An Introduction to Computational Algebraic Geometry and Commutative Algebra*. Springer-Verlag, New York, 1997.
3. W. Fulton: *Introduction to Toric Varieties*, Annals of Mathematics Studies 131, Princeton University Press, Princeton, NJ, 1993.
4. H. Hironaka: Resolution of singularities of an algebraic variety over a field of characteristic zero I, II, *Ann. of Math.* 79(2):109–203, 1964.
5. J. Howald: Multiplier ideals of monomial ideals, *Trans. Amer. Math. Soc.* 353(7):2665–2671, 2001.
6. S. Lin, B. Sturmfels and Z. Xu: Marginal likelihood integrals for mixtures of independence models, *J. Mach. Learn. Res.* 10:1611–1631, 2009.
7. S. Lin: *Algebraic methods for evaluating integrals in Bayesian statistics*, PhD dissertation, Dept. Mathematics, UC Berkeley (2011).
8. R. Pemantle and M. Wilson: Twenty combinatorial examples of asymptotics derived from multivariate generating functions, *SIAM Review* 50:199–272, 2008.
9. R. Pemantle and M. Wilson: Asymptotic expansions of oscillatory integrals with complex phase, *Algorithmic probability and combinatorics*, Contemp. Math. 520:221–240, Amer. Math. Soc., Providence, RI, 2010.
10. M. Saia: The integral closure of ideals and the Newton filtration, *J. Alg. Geom.* 5(1):1–11, 1996.
11. S. Watanabe: *Algebraic Geometry and Statistical Learning Theory*, Cambridge Monographs on Applied and Computational Mathematics 25, Cambridge University Press, Cambridge, 2009.