Asymptotic Approximation of Marginal Likelihood Integrals

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A Statistical Example

132 Schizophrenic Patients

- Evans-Gilula-Guttman(1989) studied schizophrenic patients for connections between recovery time (in years Y) and frequency of visits by relatives.

	$2{\leq}Y{<}10$	$10{\leq}Y{<}20$	$20{\leq}Y$	Totals
Regularly	43	16	3	62
Rarely	6	11	10	27
Never	9	18	16	43
Totals	58	45	29	**132**

- Proposed two statistical models to explain the data.

132 Schizophrenic Patients

- Model 1: Independence Model

	$2 \leq Y < 10$	$10 \leq Y < 20$	$20 \leq Y$
Regularly	$a_1 b_1$	$a_1 b_2$	$a_1 b_3$
Rarely	$a_2 b_1$	$a_2 b_2$	$a_2 b_3$
Never	$a_3 b_1$	$a_3 b_2$	$a_3 b_3$

132 Schizophrenic Patients

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- ## Model 2: Hidden Variable Model

	$2 \leq Y < 10$	$10 \leq Y < 20$	$20 \leq Y$
Regularly	$t a_1 b_1 + (1-t) c_1 d_1$	$t a_1 b_2 + (1-t) c_1 d_2$	$t a_1 b_3 + (1-t) c_1 d_3$
Rarely	$t a_2 b_1 + (1-t) c_2 d_1$	$t a_2 b_2 + (1-t) c_2 d_2$	$t a_2 b_3 + (1-t) c_2 d_3$
Never	$t a_3 b_1 + (1-t) c_3 d_1$	$t a_3 b_2 + (1-t) c_3 d_2$	$t a_3 b_3 + (1-t) c_3 d_3$

Marginal Likelihood Integrals

- In Bayesian statistics, models are selected by comparing *marginal likelihood integrals*.

$$Z = \int_\Omega \prod_{i,j} p_{ij}(\omega)^{U_{ij}} \, \varphi(\omega) d\omega$$

U_{ij} the data, Ω parameter space
$p_{ij}(\omega)$ functions parametrizing the model
$\varphi(\omega)$ prior belief about parameter space

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- e.g. for the first model,

$$Z_1 = \int_{\Delta_2} \int_{\Delta_2} a_1^{62} a_2^{27} a_3^{43} b_1^{58} b_2^{45} b_3^{29} \, da \, db$$

$a = (a_1, a_2, a_3)$, $b = (b_1, b_2, b_3)$
$\Delta_2 = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_i \geq 0, \sum_i x_i = 1\}$

Asymptotic Approximation

- In general, we want to compute

$$Z(n) = \int_\Omega \prod_{i=1}^{k} p_i(\omega)^{nq_i} \, |\varphi(\omega)| d\omega$$

n sample size

Ω compact and semianalytic

  i.e. $\Omega = \{\omega \in \mathbb{R}^d : g_1 \geq 0, \ldots, g_l \geq 0\}$, g_i real analytic on $\mathbb{R}^d$

φ nearly analytic

  i.e. $\varphi = \varphi_s \varphi_a$, φ_s positive and smooth, φ_a real analytic on Ω

p_i positive real analytic functions on Ω summing to 1

q true distribution with $q = p(\omega^*)$ for some $\omega^* \in \Omega$

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● L.-Sturmfels-Xu(2008) gave efficient algorithms for computing $Z(n)$ *exactly* for small samples n.

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- L.-Sturmfels-Xu(2008) gave efficient algorithms for computing $Z(n)$ *exactly* for small samples n.

- *Asymptotically*, as $n \to \infty$,

$$Z(n) \approx (\textstyle\prod_{i=1}^k q_i^{q_i})^n \cdot Cn^{-\lambda}(\log n)^{\theta-1}$$

In this talk, we want to compute (λ, θ).
In machine learning, λ is called the *learning coefficient* of the statistical model and θ its *multiplicity*.

Statistical Learning Theory
and Singularity Theory

Statistical Learning Theory

Define $Q(\omega) = \|p(\omega) - q\|^2 = \sum_{i=1}^{k} \left(p_i(\omega) - q_i \right)^2$.

Theorem (Watanabe)

If (λ, θ) is the learning coefficient and its multiplicity, then asymptotically

$$\int_{\Omega} e^{-nQ(\omega)} |\varphi(\omega)| d\omega \;\approx\; Cn^{-\lambda} (\log n)^{\theta-1}$$

for some constant C.

Singularity Theory

Theorem (Arnold-Gusein·Zade-Varchenko)

Let f be a real analytic function on Ω with $f(\omega^*) = 0$ for some $\omega^* \in \Omega$. If we have asymptotics

$$Z(n) = \int_\Omega e^{-n|f(\omega)|}|\varphi(\omega)|d\omega \approx Cn^{-\lambda}(\log n)^{\theta-1},$$

then λ is the smallest pole of the zeta function

$$\zeta(z) = \int_\Omega |f(\omega)|^{-z}|\varphi(\omega)|d\omega, \quad z \in \mathbb{C}$$

and θ is the multiplicity of this pole.

Example: Monomial Functions

- Let $f = \omega_1^{\kappa_1} \cdots \omega_d^{\kappa_d}$, $\varphi = \omega_1^{\tau_1} \cdots \omega_d^{\tau_d}$ and $\Omega = [0, \varepsilon]^d$.

$$\int_{[0,\varepsilon]^d} e^{-n\omega^\kappa} \omega^\tau \, d\omega = C n^{-\lambda} (\log n)^{\theta - 1}$$

Example: Monomial Functions

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$$\int_{[0,\varepsilon]^d} e^{-n\omega^\kappa} \omega^\tau \, d\omega = C n^{-\lambda} (\log n)^{\theta - 1}$$

- To find (λ, θ), we study the zeta function

$$\int_\Omega \omega^{-\kappa z + \tau} \, d\omega = \left[\frac{\omega_1^{-\kappa_1 z + \tau_1 + 1}}{-\kappa_1 z + \tau_1 + 1} \right]_0^\varepsilon \cdots \left[\frac{\omega_d^{-\kappa_d z + \tau_d + 1}}{-\kappa_d z + \tau_d + 1} \right]_0^\varepsilon$$

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- Thus, $\lambda = \min_i \left\{ \frac{\tau_i + 1}{\kappa_i} \right\}$, $\theta = \# \min_i \left\{ \frac{\tau_i + 1}{\kappa_i} \right\}$

    where $\# \min S$ is the number of times
    the minimum is attained in a set S.

Resolution of Singularities

Theorem (Hironaka)

Let f be a real analytic function at the origin with $f(0) = 0$.

Then, there exists a manifold M, a neighborhood W of the origin and a proper real analytic map $\rho : M \to W$ such that

- ρ is an isomorphism on $M \setminus (f \circ \rho)^{-1}(0)$

- $f \circ \rho$ and $|\rho'|$ are monomial functions locally at each $y \in (f \circ \rho)^{-1}(0)$

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  locally at each $y \in (f \circ \rho)^{-1}(0)$

Thus, we can find the poles of the zeta function of any f, provided we have a resolution of singularities for f.
Finding resolutions is generally a hard problem.

Marginal Likelihood Integral

$$\int_\Omega \prod_{i=1}^k p_i(\omega)^{n q_i} |\varphi(\omega)| d\omega$$

$$\approx C(\prod_{i=1}^k q_i^{q_i})^n \, n^{-\lambda} (\log n)^{\theta - 1}$$

Watanabe

Laplace Integral of Sum of Squares

$$\int_\Omega e^{-n \sum_{i=1}^k (p_i(\omega) - q_i)^2} |\varphi(\omega)| d\omega$$

$$\approx C n^{-\lambda} (\log n)^{\theta - 1}$$

Arnold et al.

Poles of a Monomial Function

$$\int \mu^{-\kappa z + \tau} d\mu$$

Hironaka

Zeta Function of Sum of Squares

(λ, θ) is smallest pole of

$$\zeta(z) = \int_\Omega |Q(\omega)|^{-z} |\varphi(\omega)| d\omega$$

Real Log Canonical Thresholds

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- $\Omega \subset \mathbb{R}^d$ compact semianalytic subset
  $\mathcal{A}_\Omega$ ring of real analytic functions on Ω
  $I = \langle f_1, \dots, f_r \rangle \subset A_\Omega$, φ nearly analytic

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- Consider the zeta function

$$\zeta(z) = \int_\Omega \left(f_1(\omega)^2 + \cdots + f_r(\omega)^2 \right)^{-z/2} |\varphi(\omega)| d\omega$$

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- Consider the zeta function

$$\zeta(z) = \int_\Omega \left(f_1(\omega)^2 + \cdots + f_r(\omega)^2 \right)^{-z/2} |\varphi(\omega)| d\omega$$

- Define $\mathrm{RLCT}_\Omega(I; \varphi) = (\lambda, \theta)$ where λ is
  the smallest pole of $\zeta(z)$ and θ its multiplicity.
  If $\zeta(z)$ does not have any poles, set $(\lambda, \theta) = (\infty, d)$.

  Call λ the *real log canonical threshold* of $(I; \varphi)$ on Ω.

Fundamental Properties

- RLCT's are independent of the choice of generators $f_1, \ldots, f_r$ for the ideal I.

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  If $\lambda \neq \infty$, then $\lambda \in \mathbb{Q}, 0 < \lambda \leq d$ and $\theta \in \mathbb{Z}, 1 \leq \theta \leq d$.

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  If $\lambda \neq \infty$, then $\lambda \in \mathbb{Q}, 0 < \lambda \leq d$ and $\theta \in \mathbb{Z}, 1 \leq \theta \leq d$.

- RLCT's are ordered.

  Define $(\lambda_1, \theta_1) < (\lambda_2, \theta_2)$ if $\lambda_1 < \lambda_2$, or $\lambda_1 = \lambda_2$ and $\theta_1 > \theta_2$.

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- RLCT's are local in nature.

$$\mathrm{RLCT}_\Omega(I; \varphi) = \min_{x \in \Omega} \mathrm{RLCT}_{\Omega_x}(I; \Omega)$$

where each Ω_x is a sufficiently small nbhd of x in Ω.

Local Properties

Because RLCT's are local, we will now assume:

Ω_0 a sufficiently small neighborhood of the origin

I an ideal of real analytic functions at the origin

φ a nearly analytic function at the origin

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Important local properties:

- RLCT's depend on the boundary structure of Ω_0.

- Formula for disjoint variables

- Formula for change of variables.

Example: Boundary Structure

Let $I = \langle y^2 - x^3 \rangle$ and $\varphi = 1$.
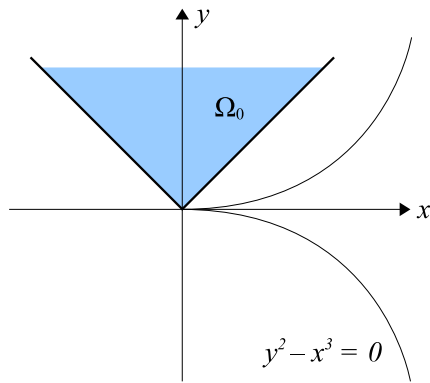
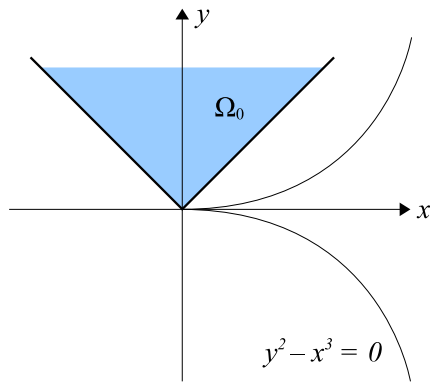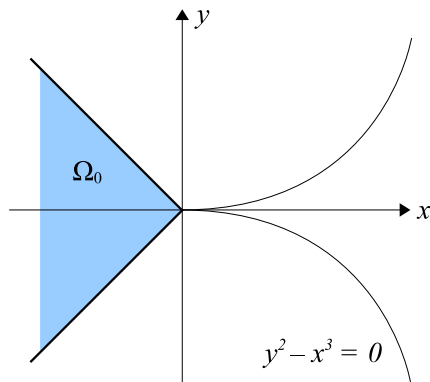- Case 1: $\Omega_0 = \{(x, y) \in \mathbb{R}^2 : 0 \leq y \leq \varepsilon, -y \leq x \leq y\}$

$$\mathrm{RLCT}_{\Omega_0}(I; \varphi) = (1, 1)$$

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- **Case 1:** $\Omega_0 = \{(x, y) \in \mathbb{R}^2 : 0 \leq y \leq \varepsilon, -y \leq x \leq y\}$

$$\mathrm{RLCT}_{\Omega_0}(I; \varphi) = (1, 1)$$

- **Case 2:** $\Omega_0 = \{(x, y) \in \mathbb{R}^2 : -\varepsilon \leq x \leq 0, x \leq y \leq -x\}$

$$\mathrm{RLCT}_{\Omega_0}(I; \varphi) = \left(\tfrac{5}{6}, 1\right)$$

Disjoint Variables

- Suppose we have disjoint sets of variables

$$x = (x_1, \ldots, x_m) \qquad\qquad y = (y_1, \ldots, y_n)$$
$$I_x = \langle f_1(x), \ldots, f_r(x) \rangle \qquad I_y = \langle g_1(y), \ldots, g_s(y) \rangle$$
$$(\lambda_x, \theta_x) = \mathrm{RLCT}_{X_0}(I_x; \varphi_x) \quad (\lambda_y, \theta_y) = \mathrm{RLCT}_{Y_0}(I_y; \varphi_y)$$

- Recall $I_x + I_y = \langle f_i, g_j \text{ for all } i, j \rangle$, $I_x I_y = \langle f_i g_j \text{ for all } i, j \rangle$

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$$(\lambda_x, \theta_x) = \mathrm{RLCT}_{X_0}(I_x; \varphi_x) \quad (\lambda_y, \theta_y) = \mathrm{RLCT}_{Y_0}(I_y; \varphi_y)$$

- Recall $I_x + I_y = \langle f_i, g_j \text{ for all } i, j \rangle$, $I_x I_y = \langle f_i g_j \text{ for all } i, j \rangle$

Proposition

$$\mathrm{RLCT}_{X_0 \times Y_0}(I_x + I_y; \varphi_x \varphi_y) = (\lambda_x + \lambda_y, \theta_x + \theta_y - 1)$$

$$\mathrm{RLCT}_{X_0 \times Y_0}(I_x I_y; \varphi_x \varphi_y) = \begin{cases} (\lambda_x, \theta_x) & \text{if } \lambda_x < \lambda_y \\ (\lambda_y, \theta_y) & \text{if } \lambda_x > \lambda_y \\ (\lambda_x, \theta_x + \theta_y) & \text{if } \lambda_x = \lambda_y \end{cases}$$

Change of Variables

- $I = \langle f_1, \ldots, f_r \rangle$

- ρ change of variables outside $\mathcal{V}(I)$

  i.e. $\rho : M \to W$ is a proper real analytic map from a manifold M to a neighborhood W of the origin that is an isomorphism on $M \setminus \rho^{-1}(\mathcal{V}(I))$

- $\rho^* I = \langle f_1 \circ \rho, \ldots, f_r \circ \rho \rangle$, $\mathcal{M} = \rho^{-1}(\Omega_0)$

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- $\rho^* I = \langle f_1 \circ \rho, \ldots, f_r \circ \rho \rangle$, $\mathcal{M} = \rho^{-1}(\Omega_0)$

Proposition

$$\mathrm{RLCT}_{\Omega_0}(I; \varphi) = \min_{y \in \rho^{-1}(0)} \mathrm{RLCT}_{\mathcal{M}_y}(\rho^* I; (\varphi \circ \rho)|\rho'|)$$

Newton Polyhedra

Newton Polyhedra

- $\omega_1, \ldots, \omega_d$ local coordinates at the origin
  I an ideal of real analytic functions at the origin

  Each $f \in I$ has a power series expansion $\sum_\alpha c_\alpha \omega^\alpha$.

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- The *Newton polyhedron* of I is the convex hull

$$\Gamma(I) = \mathrm{conv}\{\alpha + \alpha' : \sum c_\alpha \omega^\alpha \in I, c_\alpha \neq 0, \alpha' \in \mathbb{R}^d_{\geq 0}\}$$

Newton Polyhedra

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  $$\Gamma(I) = \text{conv}\{\alpha + \alpha' : \sum c_\alpha \omega^\alpha \in I, c_\alpha \neq 0, \alpha' \in \mathbb{R}^d_{\geq 0}\}$$

- $\tau = (\tau_1, \ldots, \tau_d)$ vector of non-negative integers

  The *distance* l_τ is the smallest t such that

  $$t \cdot (\tau_1 + 1, \ldots, \tau_d + 1) \in \Gamma(I)$$

  The *multiplicity* θ_τ is the codimension
  of the face of $\Gamma(I)$ at this intersection.

Example: Newton Polyhedra

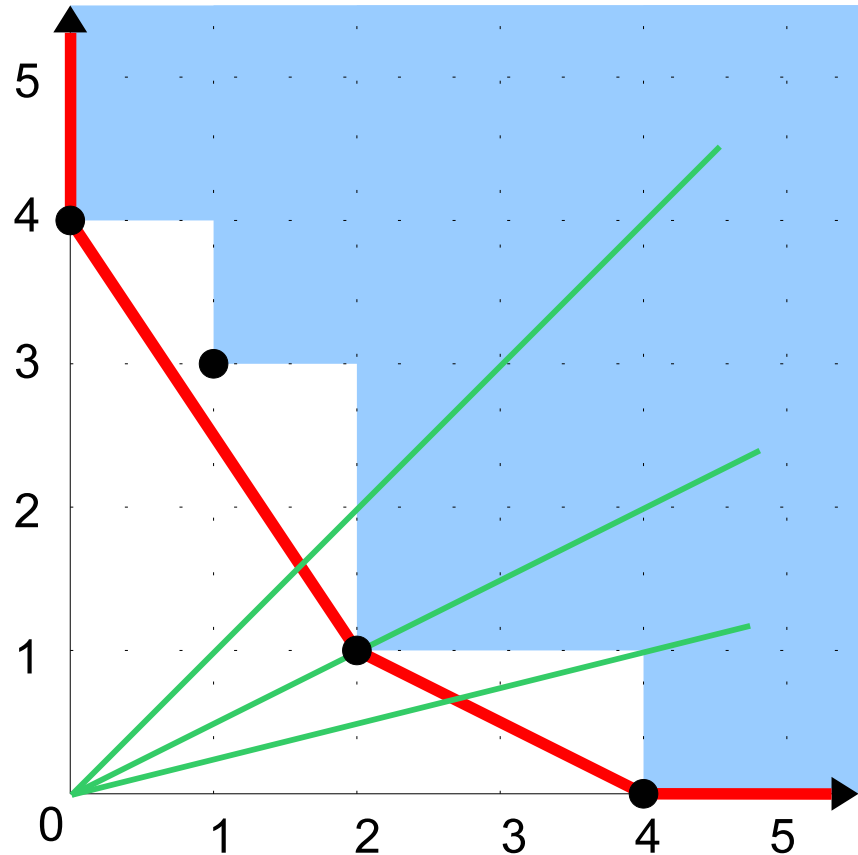$$I = \langle x^4 + x^2 y + xy^3 + y^4 \rangle$$

$$J = \langle x^4, x^2 y, xy^3, y^4 \rangle$$

Both I, J have the same Newton polyhedron.

$$l_{(0,0)} = \tfrac{8}{5}, \theta_{(0,0)} = 1$$

$$l_{(1,0)} = 1, \theta_{(1,0)} = 2$$

$$l_{(3,0)} = \tfrac{2}{3}, \theta_{(3,0)} = 1$$

Relation to RLCT

Theorem (L.)

Suppose the origin is not on the boundary of Ω.

Then, when φ is a monomial function ω^{τ},

$$\mathrm{RLCT}_{\Omega_0}(I; \omega^{\tau}) \leq (1/l_{\tau}, \theta_{\tau}).$$

Equality holds when I is a monomial ideal.

Relation to RLCT

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Remark

Equality also holds for ideals which are *nondegenerate* (a term due to Varchenko).

Back to Schizophrenic Patients

Computation

Recall $p_{ij}(t, a, b, c, d) = ta_ib_j + (1-t)c_jd_j$.
Consider $t^* = \frac{1}{2}$ and $a^* = b^* = c^* = d^* = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$.
Denote $\omega = (t, a, b, c, d)$ and $\omega^* = (t^*, a^*, b^*, c^*, d^*)$.

Let $I = \langle p_{ij}(\omega + \omega^*) - p_{ij}(\omega^*) \rangle$ and $\varphi = 1$.
We want to find $\mathrm{RLCT}_{\Omega_{\omega^*}}(I; \varphi)$.

Note that ω^* is not on the boundary of Ω.

Computation

Now, $\varphi = 1$ and I is generated by

$$p_{ij}(\omega + \omega^*) - p_{ij}(\omega^*) \text{ for all } i, j \in \{1, 2, 3\}$$

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Note that

$$p_{i1} + p_{i2} + p_{i3} = ta_i + tc_i =: p_{i0}$$
$$p_{1j} + p_{2j} + p_{3j} = tb_j + td_j =: p_{0j}$$

Let $g_{ij}(\omega)$ denote $p_{ij}(\omega + \omega^*) - p_{ij}(\omega^*)$.

Computation

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$g_{ij}(\omega)$ for all $i, j \in \{0, 1, 2\}$

Computation

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$\quad g_{ij}(\omega)$ for all $i, j \in \{0, 1, 2\}$

For $i, j \in \{1, 2\}$, we replace $g_{ij}(\omega)$ with

$\quad g_{ij}(\omega) - (d_j + d_j^*)g_{i0}(\omega) - (a_i + a_i^*)g_{0j}(\omega)$

Computation

Now, $\varphi = 1$ and I is generated by

$$g_{01}(\omega)$$

$$g_{02}(\omega)$$

$$g_{10}(\omega)$$

$$g_{20}(\omega)$$

$$g_{11}(\omega) - (d_1 + d_1^*)g_{10}(\omega) - (a_1 + a_1^*)g_{01}(\omega)$$

$$g_{12}(\omega) - (d_2 + d_2^*)g_{10}(\omega) - (a_1 + a_1^*)g_{02}(\omega)$$

$$g_{21}(\omega) - (d_1 + d_1^*)g_{20}(\omega) - (a_2 + a_2^*)g_{01}(\omega)$$

$$g_{22}(\omega) - (d_2 + d_2^*)g_{20}(\omega) - (a_2 + a_2^*)g_{02}(\omega)$$

Computation

Now, $\varphi = 1$ and I is generated by

$$g_{01}(\omega)$$
$$g_{02}(\omega)$$
$$g_{10}(\omega)$$
$$g_{20}(\omega)$$
$$g_{11}(\omega) - (d_1 + d_1^*)g_{10}(\omega) - (a_1 + a_1^*)g_{01}(\omega)$$
$$g_{12}(\omega) - (d_2 + d_2^*)g_{10}(\omega) - (a_1 + a_1^*)g_{02}(\omega)$$
$$g_{21}(\omega) - (d_1 + d_1^*)g_{20}(\omega) - (a_2 + a_2^*)g_{01}(\omega)$$
$$g_{22}(\omega) - (d_2 + d_2^*)g_{20}(\omega) - (a_2 + a_2^*)g_{02}(\omega)$$

Expanding these polynomials, we get...

Computation

Now, $\varphi = 1$ and I is generated by

$$c_1(\tfrac{1}{2} - t) + a_1(t + \tfrac{1}{2})$$

$$c_2(\tfrac{1}{2} - t) + a_2(t + \tfrac{1}{2})$$

$$d_1(\tfrac{1}{2} - t) + b_1(t + \tfrac{1}{2})$$

$$d_2(\tfrac{1}{2} - t) + b_2(t + \tfrac{1}{2})$$

$$a_1 d_1$$

$$a_1 d_2$$

$$a_2 d_1$$

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Computation

Now, $\varphi = 1$ and I is generated by

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$$d_1(\tfrac{1}{2} - t) + b_1(t + \tfrac{1}{2})$$
$$d_2(\tfrac{1}{2} - t) + b_2(t + \tfrac{1}{2})$$
$$a_1 d_1$$
$$a_1 d_2$$
$$a_2 d_1$$
$$a_2 d_2$$

Substitute $b_i = \frac{b_i' - d_i(\tfrac{1}{2} - t)}{t + \tfrac{1}{2}}$, $c_i = \frac{c_i' - a_i(t + \tfrac{1}{2})}{\tfrac{1}{2} - t}$.

The Jacobian determinant of this change of variable is 16.

Computation

Now, $\varphi = 16$ and I is generated by

$$c'_1, c'_2, b'_1, b'_2, a_1 d_1, a_1 d_2, a_2 d_1, a_2 d_2$$

Computation

Now, $\varphi = 16$ and I is generated by

$$c_1', c_2', b_1', b_2', a_1 d_1, a_1 d_2, a_2 d_1, a_2 d_2$$

This is a monomial ideal so we may use the Newton polyhedra method to compute its RLCT.

Alternatively, we can apply the formula for disjoint variables.

$$I = \langle c_1' \rangle + \langle c_2' \rangle + \langle b_1' \rangle + \langle b_2' \rangle + \Big(\langle a_1 \rangle + \langle a_2 \rangle \Big) \Big(\langle d_1 \rangle + \langle d_2 \rangle \Big)$$

Computation

Now, $\varphi = 16$ and I is generated by

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Conclusion: $\quad \mathrm{RLCT}_{\Omega_{\omega*}}(I; \varphi) = (6, 2)$

Open Questions

1. The RLCT over Ω is the minimum of RLCT's at $x \in \Omega$. How do we identify points with the minimum RLCT?

2. Is there a way to extend Newton polyhedra methods to cases where the origin is on the boundary of Ω?

Thank you for your kind attention :)

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