

# 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.

	$2 \leq Y < 10$	$10 \leq Y < 20$	$20 \leq Y$	<i>Totals</i>
Regularly	43	16	3	<i>62</i>
Rarely	6	11	10	<i>27</i>
Never	9	18	16	<i>43</i>
<i>Totals</i>	<i>58</i>	<i>45</i>	<i>29</i>	<b>132</b>

- 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

## ● Model 1: Independence Model

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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	$a_3 b_1$	$a_3 b_2$	$a_3 b_3$

## ● Model 2: Hidden Variable Model

	$2 \leq Y < 10$	$10 \leq Y < 20$	$20 \leq Y$
Regularly	$ta_1 b_1 + (1 - t)c_1 d_1$	$ta_1 b_2 + (1 - t)c_1 d_2$	$ta_1 b_3 + (1 - t)c_1 d_3$
Rarely	$ta_2 b_1 + (1 - t)c_2 d_1$	$ta_2 b_2 + (1 - t)c_2 d_2$	$ta_2 b_3 + (1 - t)c_2 d_3$
Never	$ta_3 b_1 + (1 - t)c_3 d_1$	$ta_3 b_2 + (1 - t)c_3 d_2$	$ta_3 b_3 + (1 - t)c_3 d_3$

# Marginal Likelihood Integrals

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

$$Z = \int_{\Omega} \prod_i p_i(\omega)^{U_i} \varphi(\omega) d\omega$$

$U_i$  the data,  $\Omega$  parameter space

$p_i(\omega)$  functions parametrizing the model

$\varphi(\omega)$  prior belief about parameter space

# Marginal Likelihood Integrals

● e.g. Independence Model

	$2 \leq Y < 10$	$10 \leq Y < 20$	$20 \leq Y$	<i>Totals</i>
Reg.	$a_1 b_1$ (43)	$a_1 b_2$ (16)	$a_1 b_3$ (3)	(62)
Rarely	$a_2 b_1$ (6)	$a_2 b_2$ (11)	$a_2 b_3$ (10)	(27)
Never	$a_3 b_1$ (9)	$a_3 b_2$ (18)	$a_3 b_3$ (16)	(43)
<i>Totals</i>	(58)	(45)	(29)	

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

$$a = (a_1, a_2, a_3), b = (b_1, b_2, b_3)$$

$$\Delta_2 = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_i \geq 0, \sum_i x_i = 1\}$$

# Asymptotic Approximation

- Setting  $U_i = nq_i$ , we want to compute

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

$n$  sample size

$q$  true distribution lying in  $p(\Omega)$

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- L.-Sturmfels-Xu(2008) gave efficient algorithms for computing  $Z(n)$  *exactly* for small samples  $n$ .
- *Asymptotically*, as  $n \rightarrow \infty$ ,

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

In this talk, we want to compute  $(\lambda, \theta)$ .

In machine learning,  $\lambda$  is called the *learning coefficient* of the statistical model and  $\theta$  its *multiplicity*.

# Statistical Learning Theory and Singularity Theory

# Statistical Learning Theory

## Theorem (Watanabe)

Asymptotically, if

$$\int_{\Omega} \prod_{i=1}^k p_i(\omega)^{nq_i} |\varphi(\omega)| d\omega \approx C_1 n^{-\lambda} (\log n)^{\theta-1} \cdot \left( \prod_{i=1}^k q_i^{q_i} \right)^n,$$

then

$$\int_{\Omega} e^{-nQ(\omega)} |\varphi(\omega)| d\omega \approx C_2 n^{-\lambda} (\log n)^{\theta-1}$$

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

# Singularity Theory

## Theorem (Arnold-Gusein-Zade-Varchenko)

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

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

then  $\lambda$  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  $\theta$  is the multiplicity of this pole.

# Example: Monomial Functions

• Let  $f = \omega_1^{\kappa_1} \cdots \omega_d^{\kappa_d}$  and  $\varphi = \omega_1^{\tau_1} \cdots \omega_d^{\tau_d}$ .

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

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- To find  $(\lambda, \theta)$ , we study the zeta function

$$\int_{[0,\varepsilon]^d} \omega^{-\kappa z + \tau} d\omega = \left[ \frac{\omega_1^{-\kappa_1 z + \tau_1 + 1}}{-\kappa_1 z + \tau_1 + 1} \right]_0^\varepsilon \cdots \left[ \frac{\omega_d^{-\kappa_d z + \tau_d + 1}}{-\kappa_d z + \tau_d + 1} \right]_0^\varepsilon$$

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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  $\rho : M \rightarrow W$  such that

- $\rho$  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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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

$$\int_{\Omega} \prod_{i=1}^k p_i(\omega)^{nq_i} |\varphi(\omega)| d\omega$$
$$\approx C (\prod_{i=1}^k q_i^{q_i})^n n^{-\lambda} (\log n)^{\theta-1}$$

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

$(\lambda, \theta)$  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  $\Omega$   
 $I = \langle f_1, \dots, f_r \rangle \subset \mathcal{A}_\Omega$ ,  $\varphi$  nearly analytic

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- Consider the zeta function

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

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

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

# Fundamental Properties

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

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- RLCT's are positive rational numbers.
- RLCT's are local in nature.

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

where each  $\Omega_x$  is a sufficiently small nbhd of  $x$  in  $\Omega$   
and  $(\lambda_1, \theta_1) < (\lambda_2, \theta_2)$  if  $\lambda_1 < \lambda_2$ , or  $\lambda_1 = \lambda_2$  and  $\theta_1 > \theta_2$ .

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- RLCT's depend on the boundary structure of  $\Omega_x$ .

# Fundamental Properties

- Formula for disjoint variables

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

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

# Fundamental Properties

## ● Formula for disjoint variables

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## ● Formula for change of variables

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

# Newton Polyhedra

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- $\omega_1, \dots, \omega_d$  local coordinates at the origin  
 $I$  an ideal of real analytic functions at the origin  
Each  $f \in I$  has a power series expansion  $\sum_{\alpha} c_{\alpha} \omega^{\alpha}$ .

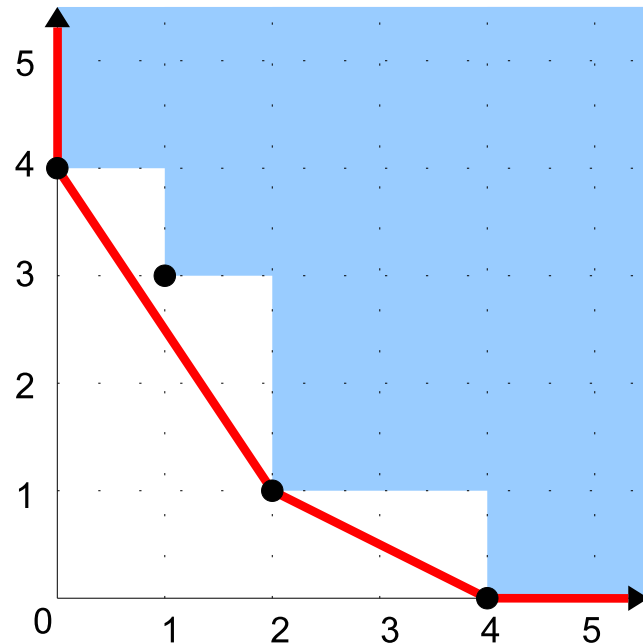
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 Each  $f \in I$  has a power series expansion  $\sum_{\alpha} c_{\alpha} \omega^{\alpha}$ .
- The *Newton polyhedron* of  $I$  is the convex hull

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

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

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



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

The *distance*  $l_{\tau}$  is the smallest  $t$  such that

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

The *multiplicity*  $\theta_{\tau}$  is the codimension of the face of  $\Gamma(I)$  at this intersection.

# Example: Newton Polyhedra

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

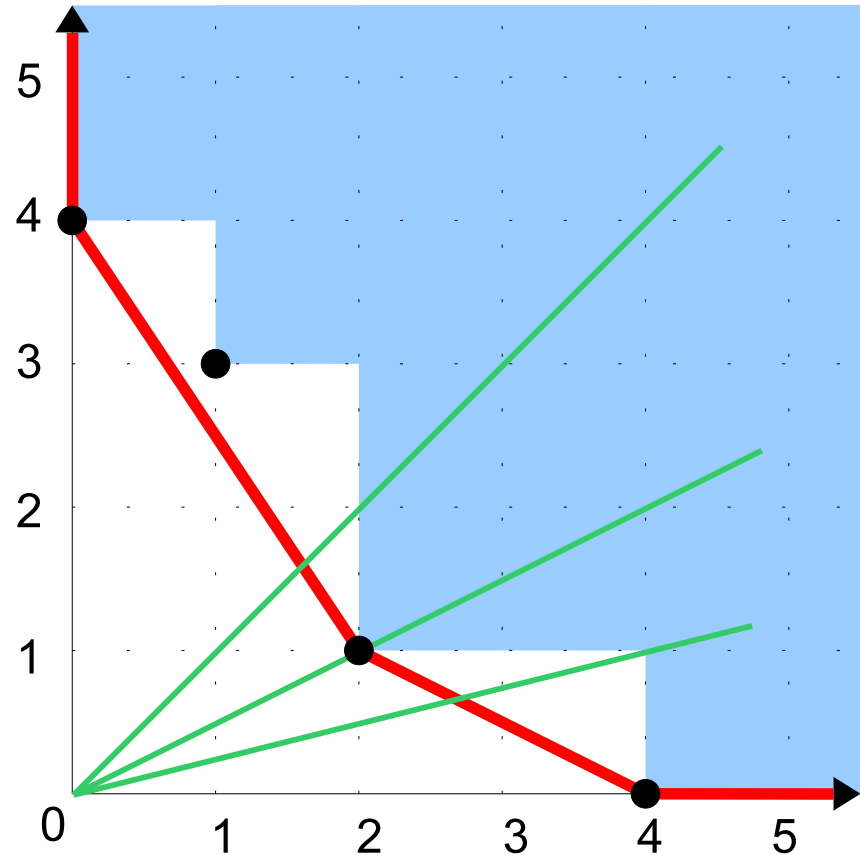
$$J = \langle x^4, x^2y, xy^3, y^4 \rangle$$

Both  $I, J$  have the same  
Newton polyhedron.

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

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

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



# Relation to RLCT

## Theorem (L.)

Suppose the origin is not on the boundary of  $\Omega$ .

Then, when  $\varphi$  is a monomial function  $\omega^\tau$ ,

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

Equality holds when  $I$  is a monomial ideal.

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Equality holds when  $I$  is a monomial ideal.

## Remark

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

**Back to Schizophrenic Patients**

# Learning Coefficients

$P = (p_{ij})$ ,  $S_i = \{\text{rank } i \text{ matrices}\}$

$S_{21} = \{p_{11} = 0; p_{12}, p_{21}, p_{22} \text{ non-zero; up to perm}\} \subset S_2$

$S_{22} = \{p_{11} = p_{22} = 0; p_{12}, p_{21} \text{ non-zero; up to perm}\} \subset S_2$

## Theorem (L.)

The learning coefficient  $(\lambda, \theta)$  of the model is

$$(\lambda, \theta) = \begin{cases} (5/2, 1) & \text{if } P \in S_1, \\ (7/2, 1) & \text{if } P \in S_2 \setminus (S_{21} \cup S_{22}), \\ (4, 1) & \text{if } P \in S_{21} \setminus S_{22}, \\ (9/2, 1) & \text{if } P \in S_{22}. \end{cases}$$

# Learning Coefficients

## Proof

Four basic techniques:

1. Changing generators for the ideal
2. Change of variables formula
3. Disjoint variables formula
4. Newton polyhedra method

(systematically peeling an onion)

# Take Home

1. Compute asymptotics using *zeta functions*.
2. When computing learning coefficients, work with RLCT of *ideals* not *functions*.
3. Newton polyhedra methods can be extended to work with monomial *amplitude functions*.

## Open Questions:

1. The RLCT over  $\Omega$  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  $\Omega$ ?

Thank you for your kind attention :)

“Asymptotic Approximation of Marginal Likelihood Integrals”

Shaowei Lin

<http://arxiv.org/abs/1003.5338>

<http://math.berkeley.edu/~shaowei/rlct.html>

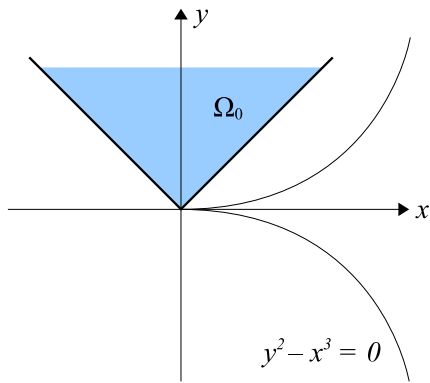
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# Example: Boundary Structure

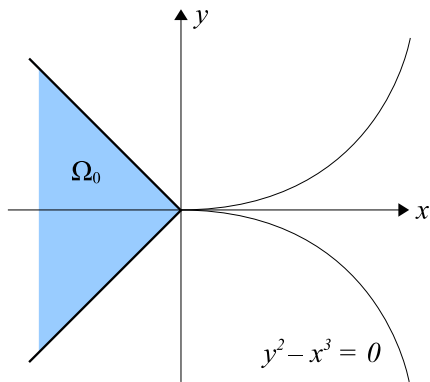
Let  $I = \langle y^2 - x^3 \rangle$  and  $\varphi = 1$ .

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



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

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



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

# Disjoint Variables

- Suppose we have disjoint sets of variables

$$x = (x_1, \dots, x_m)$$

$$y = (y_1, \dots, y_n)$$

$$I_x = \langle f_1(x), \dots, f_r(x) \rangle$$

$$I_y = \langle g_1(y), \dots, g_s(y) \rangle$$

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

- 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

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

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

# Change of Variables

- $I = \langle f_1, \dots, f_r \rangle$
- $\rho$  change of variables outside  $\mathcal{V}(I)$   
i.e.  $\rho : M \rightarrow W$  is a proper real analytic map from a manifold  $M$  to a neighborhood  $W$  of the origin that is an isomorphism on  $M \setminus \rho^{-1}(\mathcal{V}(I))$
- $\rho^*I = \langle f_1 \circ \rho, \dots, f_r \circ \rho \rangle, \mathcal{M} = \rho^{-1}(\Omega_0)$

## Proposition

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

# 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  $\text{RLCT}_{\Omega_{\omega^*}}(I; \varphi)$ .

Note that  $\omega^*$  is not on the boundary of  $\Omega$ .

# Computation

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

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

# Computation

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

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

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

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

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

# Computation

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

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

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

# 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

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Expanding these polynomials, we get...

# Computation

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

$$c_1\left(\frac{1}{2} - t\right) + a_1\left(t + \frac{1}{2}\right)$$

$$c_2\left(\frac{1}{2} - t\right) + a_2\left(t + \frac{1}{2}\right)$$

$$d_1\left(\frac{1}{2} - t\right) + b_1\left(t + \frac{1}{2}\right)$$

$$d_2\left(\frac{1}{2} - t\right) + b_2\left(t + \frac{1}{2}\right)$$

$$a_1d_1$$

$$a_1d_2$$

$$a_2d_1$$

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$$d_1\left(\frac{1}{2} - t\right) + b_1\left(t + \frac{1}{2}\right)$$

$$d_2\left(\frac{1}{2} - t\right) + b_2\left(t + \frac{1}{2}\right)$$

$$a_1 d_1$$

$$a_1 d_2$$

$$a_2 d_1$$

$$a_2 d_2$$

Substitute  $b_i = \frac{b'_i - d_i\left(\frac{1}{2} - t\right)}{t + \frac{1}{2}}$ ,  $c_i = \frac{c'_i - a_i\left(t + \frac{1}{2}\right)}{\frac{1}{2} - t}$ .

The Jacobian determinant of this change of variable is 16.

# Computation

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

$$c'_1, c'_2, b'_1, b'_2, a_1d_1, a_1d_2, a_2d_1, a_2d_2$$

# Computation

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

$$c'_1, c'_2, b'_1, b'_2, a_1d_1, a_1d_2, a_2d_1, a_2d_2$$

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.

$$I = \langle c'_1 \rangle + \langle c'_2 \rangle + \langle b'_1 \rangle + \langle b'_2 \rangle + \left( \langle a_1 \rangle + \langle a_2 \rangle \right) \left( \langle d_1 \rangle + \langle d_2 \rangle \right)$$

# Computation

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

Back