# Asymptotic Approximation of Marginal Likelihood Integrals


Shaowei Lin

shaowei@math.berkeley.edu


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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

| | $2 \le Y < 10$ | $10 \le Y < 20$ | $20 \le Y$ |
|---|---|---|---|
| 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 | $ta_1 b_1 + (1-t)c_1 d_1$ | $ta_1 b_2 + (1-t)c_1 d_2$ | $ta_1 b_3 + (1-t)c_1 d_3$ |
| 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

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|---|---|---|---|---|
| Reg. | $a_1 b_1 \quad (43)$ | $a_1 b_2 \quad (16)$ | $a_1 b_3 \quad (3)$ | $(62)$ |
| Rarely | $a_2 b_1 \quad (6)$ | $a_2 b_2 \quad (11)$ | $a_2 b_3 \quad (10)$ | $(27)$ |
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| *Totals* | $(58)$ | $(45)$ | $(29)$ | |

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

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

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

# 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 $p(\Omega)$

# Asymptotic Approximation

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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 $(\lambda, \theta)$.
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

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

then

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

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

# 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

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

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 $\rho : M \to W$ 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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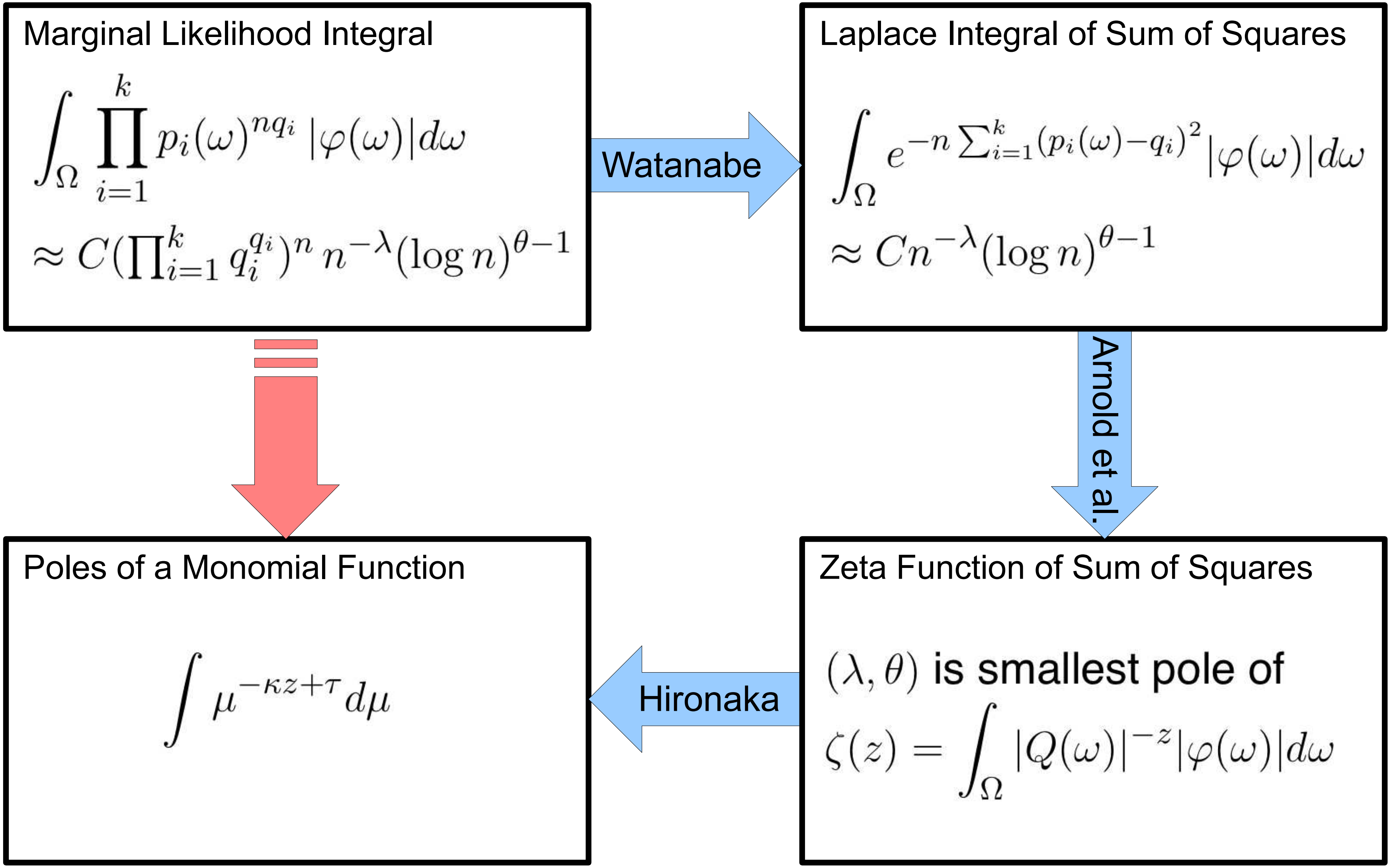
Thus, we can find the poles of the zeta function of any $f$, provided we have a resolution of singularities for $f$.
Finding resolutions is generally a hard problem.



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
$\int_\Omega e^{-n \sum_{i=1}^{k}(p_i(\omega)-q_i)^2} |\varphi(\omega)| d\omega$
$\approx Cn^{-\lambda}(\log n)^{\theta-1}$
Arnold et al.
Zeta Function of Sum of Squares
$(\lambda, \theta)$ is smallest pole of
$\zeta(z) = \int_\Omega |Q(\omega)|^{-z} |\varphi(\omega)| d\omega$
Hironaka
Poles of a Monomial Function
$\int \mu^{-\kappa z+\tau} d\mu$

# 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 $\Omega$
  $I = \langle f_1, \ldots, f_r \rangle \subset A_\Omega$, $\varphi$ nearly analytic

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- Consider the zeta function

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

- Define $\mathrm{RLCT}_\Omega(I; \varphi) = (\lambda, \theta)$ 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 $\Omega$.

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- RLCT's are local in nature.

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

  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

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

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

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\end{aligned}$$

- Formula for change of variables

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

# Newton Polyhedra

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- $\omega_1, \ldots, \omega_d$ 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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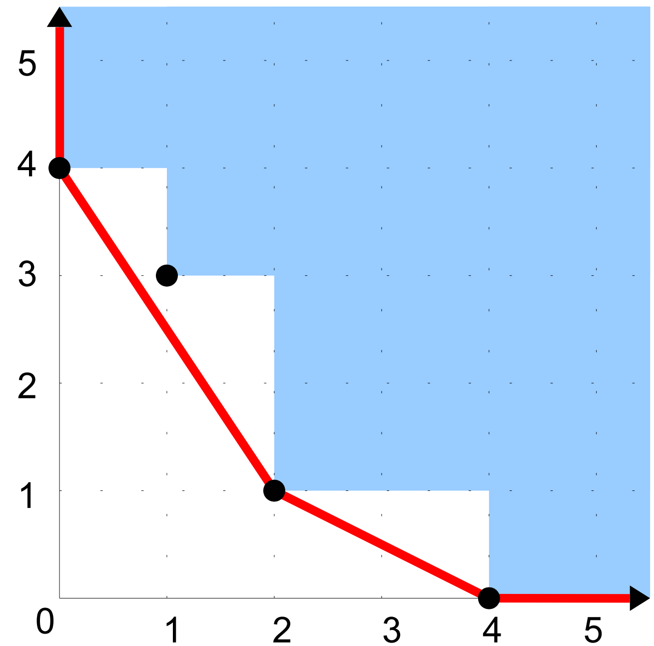
- The *Newton polyhedron* of $I$ is the convex hull

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

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

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



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

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

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

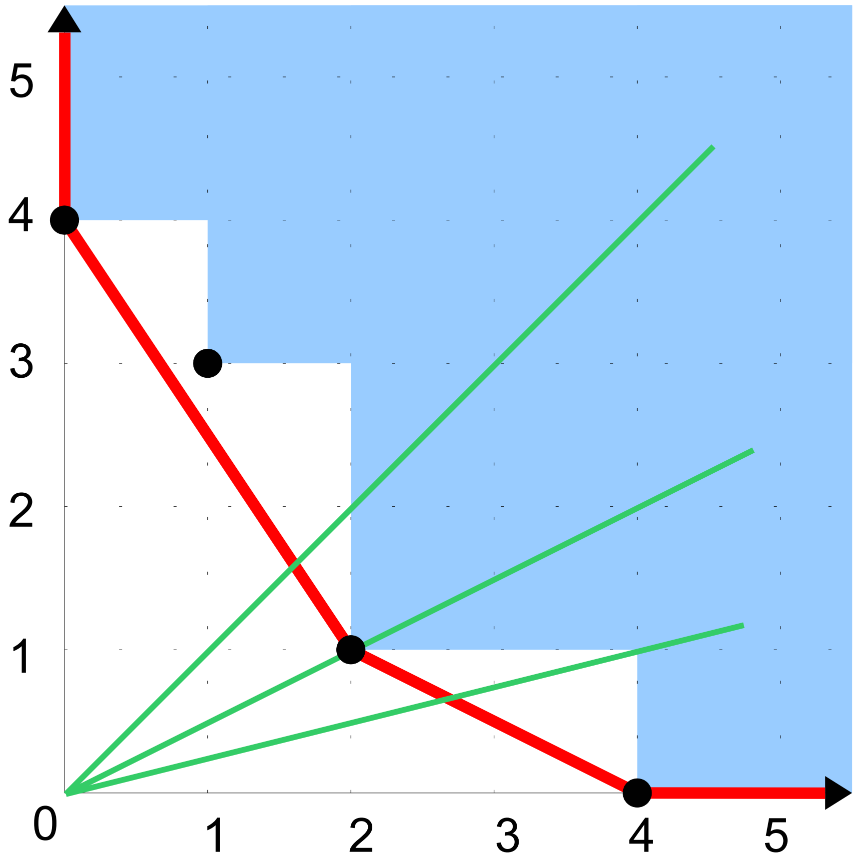
  The *multiplicity* $\theta_\tau$ is the codimension
  of the face of $\Gamma(I)$ at this intersection.

# 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 $\omega^\tau$,

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

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

$P = (p_{ij})$, $S_i = \{$rank $i$ matrices$\}$
$S_{21} = \{p_{11} = 0;\ p_{12}, p_{21}, p_{22}$ non-zero; up to perm$\} \subset S_2$
$S_{22} = \{p_{11} = p_{22} = 0;\ p_{12}, p_{21}$ 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

# References


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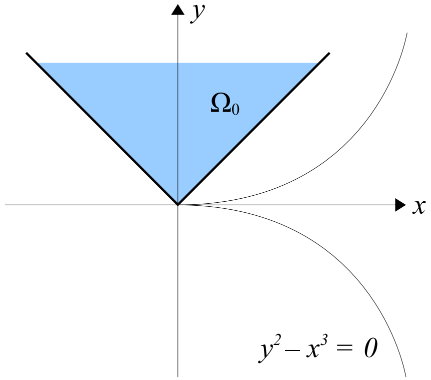
# Example: Boundary Structure

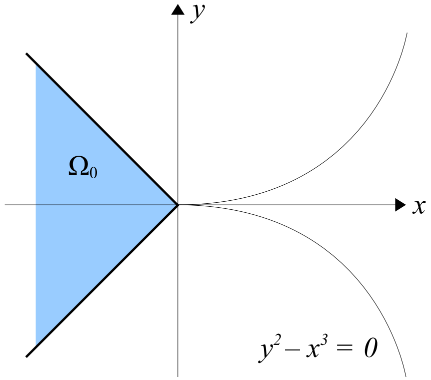
Let $I = \langle y^2 - x^3 \rangle$ and $\varphi = 1$.

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




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

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




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

Back

# Disjoint Variables

- Suppose we have disjoint sets of variables

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

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

**Proposition**

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

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

Back

# Change of Variables

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

**Proposition**

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

Back

# Computation

Recall $p_{ij}(t, a, b, c, d) = ta_i b_j + (1-t)c_j d_j$.
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 $\omega^*$ is not on the boundary of $\Omega$.

# Computation

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

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

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

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

$g_{ij}(\omega)$ 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

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

# 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

$$c_1(\tfrac{1}{2} - t) + a_1(t + \tfrac{1}{2})$$
$$c_2(\tfrac{1}{2} - t) + a_2(t + \tfrac{1}{2})$$
$$d_1(\tfrac{1}{2} - t) + b_1(t + \tfrac{1}{2})$$
$$d_2(\tfrac{1}{2} - t) + b_2(t + \tfrac{1}{2})$$
$$a_1 d_1$$
$$a_1 d_2$$
$$a_2 d_1$$
$$a_2 d_2$$

# Computation

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

$$c_1(\tfrac{1}{2} - t) + a_1(t + \tfrac{1}{2})$$
$$c_2(\tfrac{1}{2} - t) + a_2(t + \tfrac{1}{2})$$
$$d_1(\tfrac{1}{2} - t) + b_1(t + \tfrac{1}{2})$$
$$d_2(\tfrac{1}{2} - t) + b_2(t + \tfrac{1}{2})$$
$$a_1 d_1$$
$$a_1 d_2$$
$$a_2 d_1$$
$$a_2 d_2$$

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

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

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

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

$$c_1', c_2', b_1', b_2', a_1d_1, a_1d_2, a_2d_1, a_2d_2$$

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.

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

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

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