What is Singular Learning Theory?

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Why Singular Learning Theory?

Integral Asymptotics

- Laplace approximation.

$$Z(N) = \int_{\Omega} e^{-Nf(\omega)}\varphi(\omega)d\omega \approx e^{-Nf(0)} \cdot \varphi(0)\sqrt{\frac{(2\pi)^d}{\det H(0)}} \cdot N^{-d/2}$$

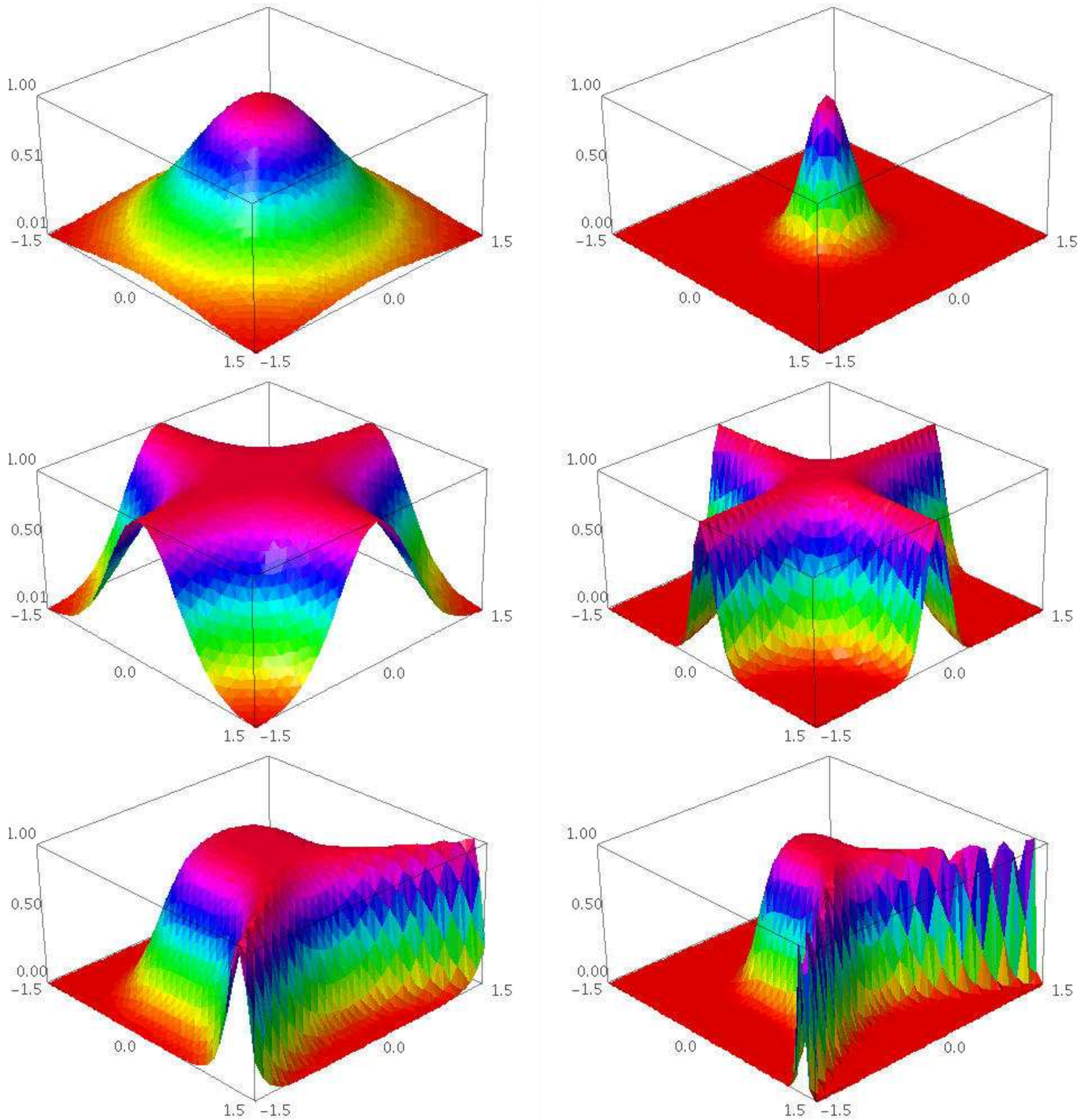
- Bayesian Information Criterion (BIC).

$$\log Z(N) \approx \left(-\sum_{i=1}^{N} \log q^*(X_i)\right) + \frac{d}{2}\log N$$

- Stirling's approximation in combinatorics.

$$N! = N^{N+1}\int_0^{\infty} e^{-N(x-\log x)}\,dx \approx N^{N+1}\sqrt{\frac{2\pi}{N}}e^{-N}$$

Plots of $z = e^{-Nf(x,y)}$ for $N = 1$ and $N = 10$



$$f(x,y) = x^2 + y^2$$

$$f(x,y) = (xy)^2$$

$$f(x,y) = (y^2 - x^3)^2$$

Integral Asymptotics

Statistical integral. $\displaystyle\int_{[0,1]^2} (1-x^2y^2)^{N/2}\,dxdy \;\approx$

$$\sqrt{\frac{\pi}{8}}N^{-\frac{1}{2}}\log N \qquad -\sqrt{\frac{\pi}{8}}\left(\frac{1}{\log 2}-2\log 2-\gamma\right)N^{-\frac{1}{2}}$$

$$-\frac{1}{4}N^{-1}\log N \qquad +\frac{1}{4}\left(\frac{1}{\log 2}+1-\gamma\right)N^{-1}$$

$$-\frac{\sqrt{2\pi}}{128}N^{-\frac{3}{2}}\log N \qquad +\frac{\sqrt{2\pi}}{128}\left(\frac{1}{\log 2}-2\log 2-\frac{10}{3}-\gamma\right)N^{-\frac{3}{2}}$$

$$0 \qquad -\frac{1}{24}N^{-2} \qquad +\cdots$$

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

Central Limit Theorem

- Sample mean.

$$S_N = \frac{1}{N}\sum_{i=1}^{N} X_i = \mu + \frac{1}{\sqrt{N}}\sigma\xi_N$$

where ξ_N converges in law to standard normal distribution.

- Log likelihood ratio.

$$K_N(\omega) = \frac{1}{N}\sum_{i=1}^{N} \log\frac{q(X_i)}{p(X_i|\omega)} = \mu^{2\kappa} - \frac{1}{\sqrt{N}}\mu^{\kappa}\xi_N(\mu)$$

where $\xi_N(\mu)$ converges in law to a Gaussian process.

Singular Learning Theory

A statistical model is *regular* if it is identifiable and its Fisher information matrix is postive definite. Behavior of regular models for large samples is well-understood, e.g. *central limit theorems*.

A model is *singular* if it is not regular. Many hidden variable models are singular. Singular learning theory teaches us how to study the *asymptotic behavior* of singular models: *by monomializing the Kullback-Leibler distance*.

Statistical Model

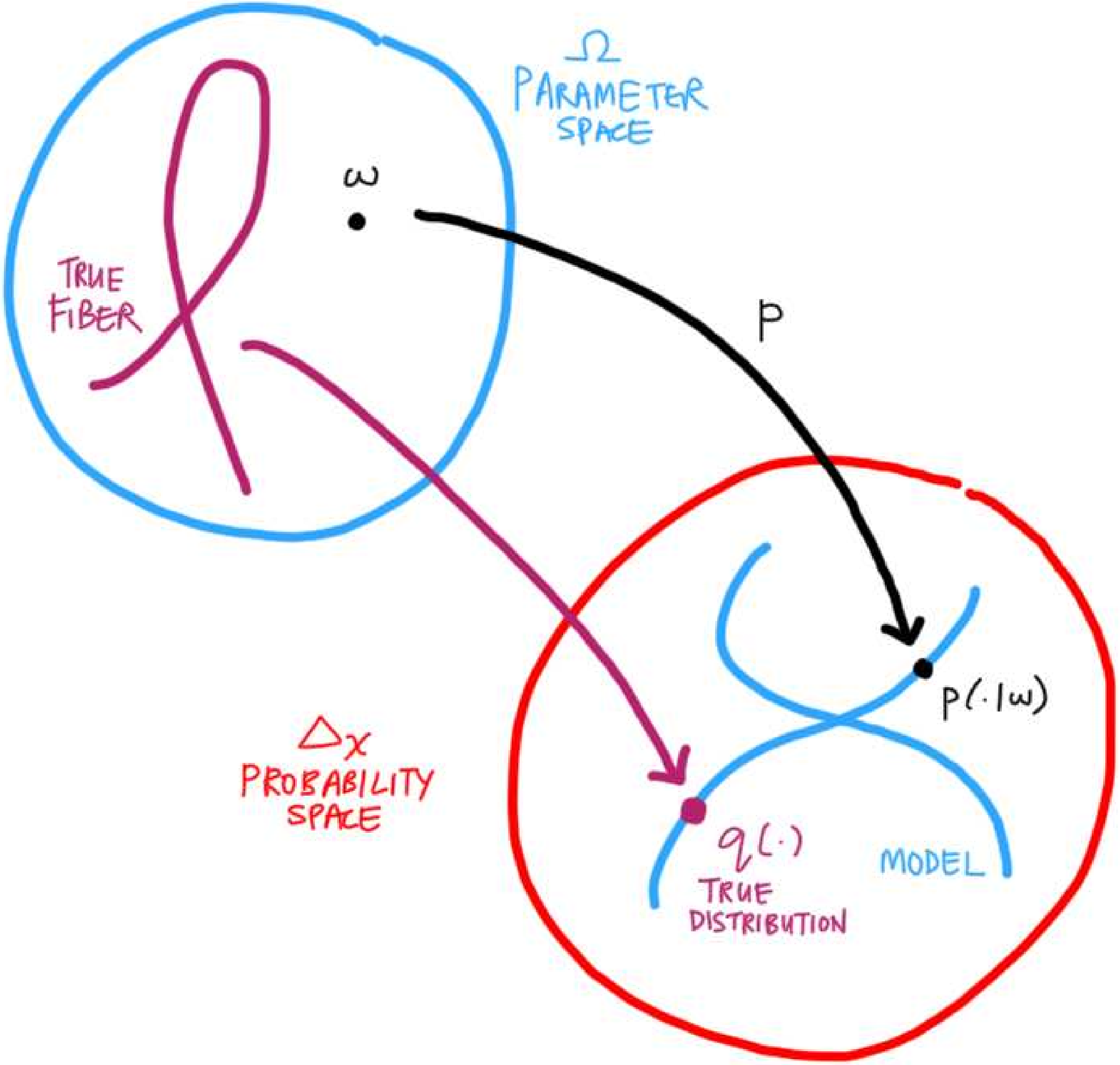
Let X be a random variable with state space $\mathcal{X}$ (e.g. $\{1, 2, \ldots, k\}$, $\mathbb{R}^k$).
Let $X_1, \ldots, X_N$ be N independent random samples of X.

Let $\mathcal{M}$ be a statistical model on $\mathcal{X}$ with parameter space Ω,
where the distribution at $\omega \in \Omega$ is denoted by $p(x|\omega)dx$
and the prior distribution on Ω is given by $\varphi(\omega)d\omega$.

In *statistical learning theory*, we are interested in using the
data $X_1, \ldots, X_N$ to select a model $\mathcal{M}$ that best describes X.
For this purpose, many *model selection criteria* (e.g. maximum
likelihood, marginal likelihood, AIC, BIC) have been designed.

Important to analyze how these criteria behave as N *grows large*.
To do this, we need to assume X has *true distribution* $q(x)dx$.
Let the *true fiber* be the set of all $\omega \in \Omega$ which map to $q(x)dx$.

Statistical Model



Kullback-Leibler distance

Given a model, recall that the *likelihood* of the data is

$$L_N(\omega) = \prod_{i=1}^{N} p(X_i|\omega).$$

To compare the model distribution with the true distribution, we have the *log likelihood ratio*

$$K_N(\omega) = \frac{1}{N} \log \frac{\prod_{i=1}^{N} q(X_i)}{\prod_{i=1}^{N} p(X_i|\omega)} = \frac{1}{N} \sum_{i=1}^{N} \log \frac{q(X_i)}{p(X_i|\omega)}.$$

In fact, the expectation of $K_N(\omega)$ over the data distribution is the *Kullback-Leibler distance*

$$K(\omega) = \int_{\mathcal{X}} q(x) \log \frac{q(x)}{p(x|\omega)} dx.$$

In statistics, this distance is an important measure of the difference between two distributions.

Regular and Singular Models

Suppose $q(x)dx$ equals $p(x|\omega_0)dx$ for some $\omega_0 \in \Omega$.

The model is *identifiable* at ω_0 if the true fiber has only one point.

The *Fisher information matrix* $I(\omega_0)$ is the Hessian matrix of the KL distance $K(\omega)$ at ω_0. This matrix is always *positive semidefinite*.

A model is *regular* if it is identifiable and the Fisher information matrix $I(\omega)$ is *positive definite* at all $\omega \in \Omega$.

A model is *singular* if it is not regular. In particular, singular models are either nonidentifiable, or $\det I(\omega) = 0$ for some $\omega \in \Omega$.

The asymptotic behavior of regular models is well-understood.
[See Schwarz(1978), Haughton(1988), Lauritzen(1996).]
Unfortunately, many important models in learning theory are singular.

Asymptotic Behavior

To analyze the *asymptotic behavior* of model selection criteria, we often need to understand the *log likelihood ratio* $K_N(\omega)$.

e.g. Marginal likelihood

$$Z_N = \int_\Omega \prod_{i=1}^N p(X_i|\omega)\varphi(\omega)d\omega = \prod_{i=1}^N q(X_i) \cdot \int_\Omega e^{-NK_N(\omega)}\varphi(\omega)d\omega$$

e.g. For regular models, the Bayesian Information Criterion (BIC) uses the approximation $-\log Z_N \approx -\log L_N^* + \frac{d}{2}\log N$ for model selection. Here, L_N^* is the maximum likelihood and d the model dimension.

Watanabe showed that the *log likelihood ratio* $K_N(\omega)$ can be put in a nice standard form if we resolve the singularities of the *Kullback-Leibler distance* $K(\omega)$.

Resolution of Singularities

Watanabe's insight: find a change of variables $\rho : \mathscr{M} \to \Omega$
such that $K(\omega)$ becomes *locally monomial* on the *manifold* $\mathscr{M}$.

Such a change of variables always exists, due to a deep theorem in algebraic geometry known as *resolution of singularities*. [Proved in 1964, this theorem won Hironaka the Fields Medal.]

Standard Form of Log Likelihood Ratio (Watanabe)

Given mild conditions on the model $\mathcal{M}$, there exists a change of variable $\rho : \mathscr{M} \to \Omega$ such that (μ^κ denotes $\mu_1^{\kappa_1} \cdots \mu_d^{\kappa_d}$)

$$K_N(\rho(\mu)) = \mu^{2\kappa} - \frac{1}{\sqrt{N}} \mu^\kappa \xi_N(\mu)$$

where $\xi_N(\mu)$ converges in law to a Gaussian process on $\mathscr{M}$.

This is the *generalized Central Limit Theorem* for singular models.

Learning Coefficient

Define empirical entropy $S_N = -\frac{1}{N}\sum_{i=1}^{N} \log q(X_i)$.

Convergence of stochastic complexity (Watanabe)

Given mild conditions on the model $\mathcal{M}$, the *stochastic complexity* $-\log Z_N$ has the asymptotic expansion

$$-\log Z_N = NS_N + \lambda \log N - (\theta - 1) \log \log N + F_N^R$$

where F_N^R converges in law to a random variable. Moreover, λ is the smallest pole, and θ its order, of the zeta function

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

This is the *generalized BIC* for singular models.

We call λ the *learning coefficient* of the model $\mathcal{M}$ at the true distribution, and θ its *order*. We compute them by *monomializing* $K(\omega)$ and $\varphi(\omega)$.

Computation

Suppose $K(\omega) = \omega_1^{\kappa_1} \cdots \omega_d^{\kappa_d}$, $\varphi(\omega) = \omega_1^{\tau_1} \cdots \omega_d^{\tau_d}$ and $\Omega = [0, \varepsilon]^d$.

Then, the zeta function is

$$\begin{aligned}\zeta(z) &= \int_{[0,\varepsilon]^d} \omega_1^{-\kappa_1 z + \tau_1} \cdots \omega_d^{-\kappa_d z + \tau_d} \, d\omega \\ &= \frac{\varepsilon^{-\kappa_1 z + \tau_1 + 1}}{-\kappa_1 z + \tau_1 + 1} \cdots \frac{\varepsilon^{-\kappa_d z + \tau_d + 1}}{-\kappa_d z + \tau_d + 1}\end{aligned}$$

The poles of this function are $(\tau_i + 1)/\kappa_i$ for each i.

Thus, the learning coefficient is given by

$$\lambda = \min_i \frac{\tau_i + 1}{\kappa_i}$$

and its order θ is the number of times this minimum is attained.

The most *difficult* computation
in singular learning
is *finding* a change of variables
which monomializes $K(\omega)$.

Algebraic Geometry

Linear Algebra is the study of
systems of *linear* equations.

Commutative Algebra is the study of
systems of *polynomial* equations.

Algebraic Geometry is the study of
solutions of systems of polynomial equations.

Simple Example

Polynomial system $\{y - x^2, y\} \subset \mathbb{C}[x, y]$ $\longleftrightarrow$ Solution set (*variety*) $V = \{(0, 0)\} \subset \mathbb{C}^2$

Because the polynomials $y - x^2$ and y vanish on V, so do all other polynomials of the form

$$p(x, y) = (y - x^2)\, p_1(x, y) + (y)\, p_2(x, y).$$

This infinite set of polynomials is the *ideal* $I = \langle y - x^2, y \rangle$.

Is $x^2 \in I$? Is $x \in I$?

Ideals: generated by addition, polynomial multiplication.
Vector spaces: generated by addition, scalar multiplication.

Ideals and Varieties

Let $\mathcal{R} = \mathbb{C}[x_1, x_2, \ldots, x_d]$ be a polynomial ring.

Given a subset $I \subset \mathcal{R}$, we define the *variety*

$$\mathcal{V}(I) = \{x \in \mathbb{C}^d \mid f(x) = 0 \text{ for all } f \in I\}.$$

Given a subset $V \subset \mathbb{C}^d$, we define the *ideal*

$$\mathcal{I}(V) = \{f \in \mathcal{R} \mid f(x) = 0 \text{ for all } x \in V\}.$$

The *algebraic closure* of V is the set $\overline{V} = \mathcal{V}(\mathcal{I}(V))$.

The *radical* of I is the set

$$\sqrt{I} = \{f \mid f^n \in I \text{ for some positive integer } n\}.$$

Fundamental Theorems

Hilbert Basis Theorem

Every ideal in $\mathbb{C}[x_1, \ldots, x_d]$ is finitely generated.

Hilbert's Nullstellensatz

$$\mathcal{I}(\mathcal{V}(I)) = \sqrt{I}$$

There is a bijective correspondence between radical ideals in $\mathbb{C}[x_1, \ldots, x_d]$ and varieties in $\mathbb{C}^d$.

BIG IDEA: Study varieties by studying their ideals.

Gröbner Bases

Every system of linear equations has a *row echelon form*, which is computed using *Gaussian elimination*.

Every system of polynomial equations has a *Gröbner basis*, which is computed using *Buchberger's algorithm*.

Determine ideal membership (e.g. Is $x^2 \in I$? Is $x \in I$?), dimension, degree, number of solutions, radicals, irreducible components, elimination of variables, etc.

Textbook:
"Ideals, Varieties, and Algorithms," Cox-Little-O'Shea(1997)

Software: `Macaulay2`, `Singular`, `Maple`, etc.

Real Log Canonical Thresholds

The Kullback-Leibler distance $K(\omega)$
is a *nonpolynomial* function that is
computationally difficult to monomialize.

Many singular models, however,
are regular models whose parameters are
polynomial functions of new parameters.

We want to *exploit* this polynomiality
in computing their learning coefficients.

Regularly Parametrized Models

A model $\mathcal{M}$ is *regularly parametrized* if it can be expressed as a regular model whose parameters $u = (u_i)$ are analytic functions $u_i(\omega)$ of new parameters $\omega = (\omega_i)$.

e.g. Discrete models $(p_1(\omega), p_2(\omega), \ldots, p_k(\omega))$
Gaussian models $X \sim \mathcal{N}(\mu, \Sigma)$, $\mu = (\mu_i(\omega))$, $\Sigma = (\sigma_{ij}(\omega))$

Suppose the true distribution lies in the model $\mathcal{M}$, i.e. $q(x) = p(x|\omega^*)$ for some $\omega^* \in \Omega$.

Define the *fiber ideal* $I = \langle u_i(\omega) - u_i(\omega_i^*)$ for all $i\rangle$.
It is the ideal of the *true fiber* $V = \{\omega \in \Omega \mid q(x) = p(x|\omega)$ for all $x\}$.

Real Log Canonical Thresholds

In algebraic geometry, the *real log canonical threshold* of an ideal $\langle f_1(\omega), \ldots, f_k(\omega)\rangle$ is the pair (λ, θ) where λ is the smallest pole of the zeta function

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

and θ its order. We denote $(\lambda, \theta) = \mathrm{RLCT}_\Omega(I; \varphi)$.

- This definition is independent of the choice of generators for I.
- Fix I, Ω and φ. For each point $x \in \Omega$, there exists a sufficiently small open neighborhood Ω_x of x in Ω such that $\mathrm{RLCT}_U(I; \varphi)$ is the same for all open neighborhoods U of x contained in Ω_x.
- We order the pairs (λ, θ) by the value of $\lambda \log N - (\theta - 1) \log\log N$ for sufficiently large N.

Exploiting Polynomiality

Theorem (L.)

Let $\mathcal{M}$ be a regularly parametrized model, and let the true distribution $q(x)dx$ be in $\mathcal{M}$. Given mild conditions on $\mathcal{M}$, the learning coefficient λ and its order θ of the model is given by

$$(2\lambda, \theta) = \min_{x \in \mathcal{V}(I)} \mathrm{RLCT}_{\Omega_x}(I; \varphi)$$

where I is the fiber ideal at the true distribution and $\mathcal{V}(I) \subset \Omega$ is the true fiber.

Newton Polyhedra

Given an ideal $I \subset \mathbb{R}[\omega_1, \ldots, \omega_d]$,

1. Plot $\alpha \in \mathbb{R}^d$ for each monomial ω^α appearing in some $f \in I$.
2. Take the convex hull $\mathcal{P}(I)$ of all plotted points.

This convex hull $\mathcal{P}(I)$ is the *Newton polyhedron* of I.

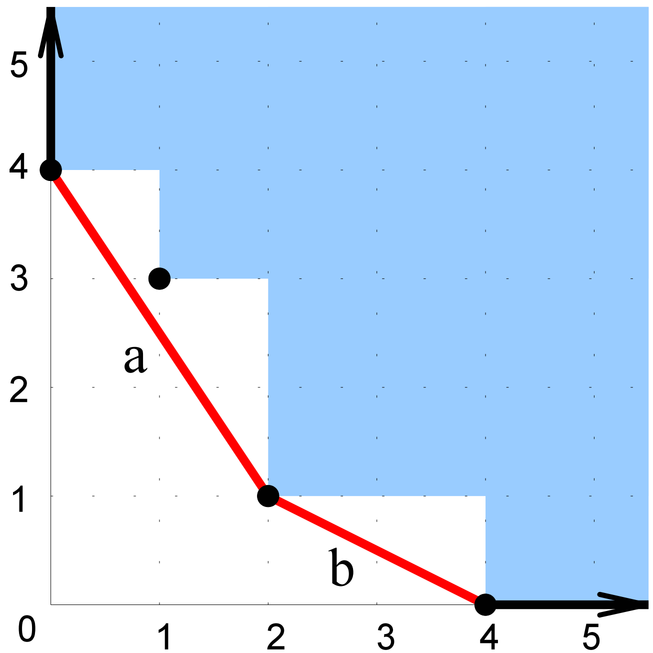
Given a vector $\tau \in \mathbb{Z}^d_{\geq 0}$, define

1. *τ-distance* l_τ : smallest $t \geq 0$ such that $t(\tau_1 + 1, \ldots, \tau_d + 1) \in \mathcal{P}(I)$.
2. *multiplicity* θ_τ : codimension of face of $\mathcal{P}(I)$ at this intersection.

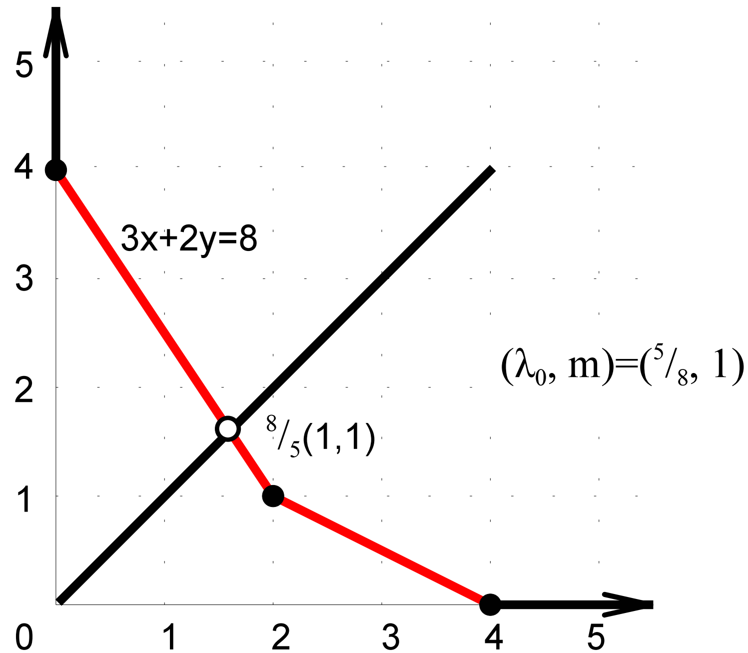
Newton Polyhedra

Let $I = \langle x^4, x^2y, xy^3, y^4 \rangle$ and $\tau = (0,0)$.

Newton polyhedron



τ-distance



The τ-distance is $l_\tau = 8/5$ and the multiplicity is $\theta_\tau = 1$.

Bounding the RLCT

Theorem (L.)

Let $I \subset \mathbb{R}[\omega_1, \ldots, \omega_d]$ be a finitely generated ideal, and $U \subset \mathbb{R}^d$ a sufficiently small nbhd of the origin. Then,

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

where l_τ is the τ-distance of the Newton polyhedron $\mathcal{P}(I)$ and θ_τ its multiplicity. Equality occurs when I is a monomial ideal.

Using this theorem, we can compute the RLCT of *any* ideal by monomializing the ideal.

Examples

Example 1: Bayesian Information Criterion

When the model is regular, the fiber ideal is $I = \langle \omega_1, \ldots, \omega_d \rangle$.
Using Newton polyhedra, the RLCT of this ideal is $(d, 1)$.

By our theorem, the learning coefficient is $(\lambda, \theta) = (d/2, 1)$.
By Watanbe's theorem, the stochastic complexity is asymptotically

$$NS_N + \frac{d}{2} \log N.$$

This formula is the *Bayesian Information Criterion* (BIC).

Examples

Example 2: **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**

They wanted to find out if the data can be explained by a *naïve Bayesian network* with two hidden states (e.g. male and female).

Examples

Example 2: 132 Schizophrenic Patients

The model is parametrized by $(t, a, b, c, d) \in \Delta_1 \times \Delta_2 \times \Delta_2 \times \Delta_2 \times \Delta_2$.

	$2 \leq Y < 10$	$10 \leq Y < 20$	$20 \leq Y$
Regularly	$ta_1b_1 + (1-t)c_1d_1$	$ta_1b_2 + (1-t)c_1d_2$	$ta_1b_3 + (1-t)c_1d_3$
Rarely	$ta_2b_1 + (1-t)c_2d_1$	$ta_2b_2 + (1-t)c_2d_2$	$ta_2b_3 + (1-t)c_2d_3$
Never	$ta_3b_1 + (1-t)c_3d_1$	$ta_3b_2 + (1-t)c_3d_2$	$ta_3b_3 + (1-t)c_3d_3$

As a model selection criteria, we compute the *marginal likelihood* of this model, given the above data and a uniform prior on the parameter space.

Examples

Example 2: **132 Schizophrenic Patients**

Lin-Sturmfels-Xu(2009) computed this integral *exactly*.
It is the rational number with numerator

$$
\begin{gathered}
27801948853106338912064360032498932910387614080 5\\
28524283958209256935726588667532284587409752803 3\\
9949306971310363319990693940571118083756885373 7
\end{gathered}
$$

and denominator

$$
\begin{gathered}
12288402873591935400678094796599848745442833177572204\\
50448819979286456995185542195946815073112429169997801\\
33503900169921912167352239204153786645029153951176422\\
43298328046163472261962028461650432024356339706541132\\
34375318471880274818667657423749120000000000000000.
\end{gathered}
$$

Examples

Example 2: 132 Schizophrenic Patients

We want to approximate the integral using asymptotic methods.
The EM algorithm gives us the *maximum likelihood distribution*

$$q = \frac{1}{132}\begin{pmatrix} 43.002 & 15.998 & 3.000 \\ 5.980 & 11.123 & 9.897 \\ 9.019 & 17.879 & 16.102 \end{pmatrix}.$$

Compare this distribution with the data

$$\begin{pmatrix} 43 & 16 & 3 \\ 6 & 11 & 10 \\ 9 & 18 & 16 \end{pmatrix}.$$

We use the ML distribution as the *true distribution* for our approximations.

Examples

Example 2: **132 Schizophrenic Patients**

Recall that stochastic complexity $= -\log$ (marginal likelihood).

- The BIC approximates the stochastic complexity as
$$NS_N + \frac{9}{2}\log N.$$
- By computing the RLCT of the fiber ideal, our approximation is
$$NS_N + \frac{7}{2}\log N.$$
- Summary:

	Stochastic Complexity
Exact	273.1911759
BIC	278.3558034
RLCT	275.9144024

“Algebraic Methods for Evaluating Integrals in Bayesian Statistics”

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

(PhD dissertation, May 2011)

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