Understanding the Curse of Singularities in Machine Learning

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UC Berkeley Statistics

Sparsity Penalties
- Linear Regression
- Param Estimation
- Laplace Approx
- Curse of Singularities
- Singular Model
- Learning Coefficient
- Faithfulness
- Higher Order

Singular Learning

Integral Asymptotics

Sparsity Penalties

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Linear Regression

Random variables $Y \in \mathbb{R}, X \in \mathbb{R}^d$ satisfy

$$Y = \omega \cdot X + \varepsilon$$

Parameters $\omega \in \mathbb{R}^d$; noise $\varepsilon \in \mathcal{N}(0,1)$; data $(Y_i, X_i), i = 1 .. N$.

- Commonly computed quantities
  - MLE $\quad \operatorname{argmin}_\omega \sum_{i=1}^N |Y_i - \omega \cdot X_i|^2$
  - Penalized MLE $\quad \operatorname{argmin}_\omega \sum_{i=1}^N |Y_i - \omega \cdot X_i|^2 + \pi(\omega)$
- Commonly used penalties
  - LASSO $\quad \pi(\omega) = |\omega|_1 \cdot \beta$
  - Bayesian Info Criterion (BIC) $\quad \pi(\omega) = |\omega|_0 \cdot \log N$
  - Akaike Info Criterion (AIC) $\quad \pi(\omega) = |\omega|_0 \cdot 2$
- Common applications
  - Parameter estimation
  - Model selection (e.g. which entries in ω are nonzero?)

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Parameter Estimation

- *Parameter estimation is a form of model selection!* For each parameter u, we define a model and compute its likelihood.
- MLE: assume data generated by true parameter $u \in \mathbb{R}^d$.

$$L(u) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2} \sum_{i=1}^{N} |Y_i - u \cdot X_i|^2)$$

- LASSO: assume data generated by true parameter $u \in \mathbb{R}^d$ which is chosen via a Laplacian prior.

$$L(u) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2} \sum_{i=1}^{N} |Y_i - u \cdot X_i|^2) \exp(-\frac{1}{2}\beta|u|_1)$$

- *Integrated likelihood*: each sample is generated by independent parameters chosen via prior $\varphi(\omega)$ on small nbhd Ω_u of $u \in \mathbb{R}^d$.

$$Z(u) = \int_{\Omega_u} \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2} \sum_{i=1}^{N} |Y_i - \omega \cdot X_i|^2) \, \varphi(\omega) d\omega$$

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Laplace Approximation

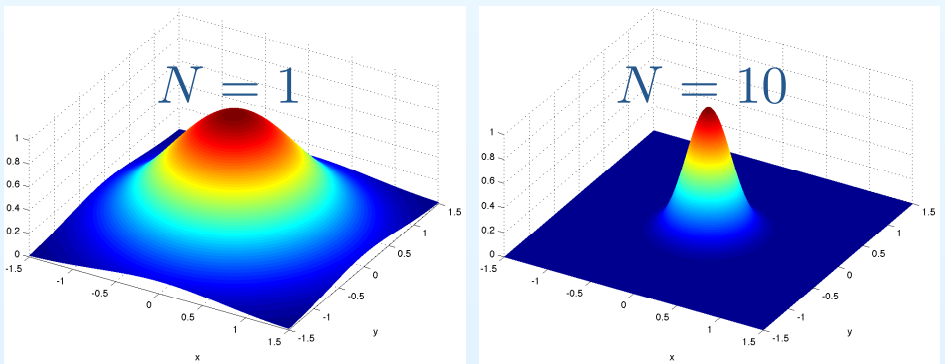
- Let $f(\omega) = \frac{1}{2N} \sum_{i=1}^{N} |Y_i - \omega \cdot X_i|^2$ so we can write

$$Z(u) = \frac{1}{\sqrt{2\pi}} \int_{\Omega_u} e^{-Nf(\omega)} \varphi(\omega) d\omega.$$

- *Laplace approximation*: If $f(\omega)$ is uniquely minimized at u and the Hessian $\partial^2 f(u)$ is full rank, then asymptotically

$$-\log Z(u) \approx Nf(u) + \frac{\dim \Omega_u}{2} \log N + O(1)$$

as sample size $N \to \infty$. This approximation gives us the BIC.



Graphs of $e^{-Nf(\omega)}$ for different N. Integral = Volume under graph.

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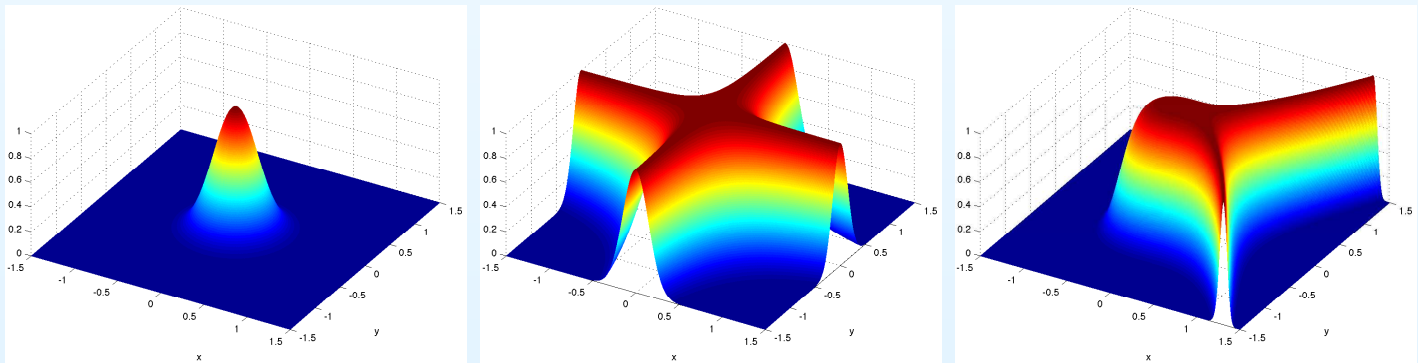
Curse of Singularities

- The AIC, where the idea is to minimize the *Kullback-Leibler distance*, can also be derived using integral asymptotics.
- For *smooth* models i.e. $\partial^2 f(u)$ is full rank, Laplace approx works well even if parameter space $\mathbb{R}^d$ has high dimension.
- But many models in machine learning are *singular*, e.g. mixtures, neural networks, hidden variables.
- How do we study the asymptotics of integrals with singularities?



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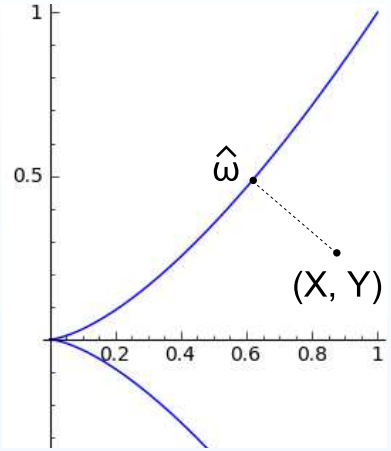
Integral Asymptotics

Example: Singular Model

$$X \sim \mathcal{N}(\omega^2, 1), \quad Y \sim \mathcal{N}(\omega^3, 1)$$
$$\text{data } (X_i, Y_i), i = 1 .. N$$
$$\text{parameter } \omega \in \mathbb{R}, \text{ mean } (\bar{X}, \bar{Y})$$



- MLE: $\operatorname{argmin}_\omega |\omega^2 - \bar{X}|^2 + |\omega^3 - \bar{Y}|^2$
  BIC performs poorly when MLE is close to 0.
- Put prior $\varphi(\omega)$ on small nbhd Ω_u of true parameter $u \in \mathbb{R}$.

$$Z(u) = \frac{1}{2\pi} \int_{\Omega_u} \exp(-\frac{1}{2} \sum_{i=1}^{N} |\omega^2 - X_i|^2 + |\omega^3 - Y_i|^2)\, \varphi(\omega) d\omega$$

- According to *Singular Learning Theory*, asymptotically

$$-\log Z(u) \approx \frac{1}{2} \sum_{i=1}^{N} (u^2 - X_i)^2 + (u^3 - Y_i)^2 + \pi(u) + O_p(1)$$

where $\pi(u) = \frac{1}{4} \log N$ if $u = 0$; otherwise $\pi(u) = \frac{1}{2} \log N$.

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Learning Coefficients

- Given $u \in \Omega$, there exist a small nbhd Ω_u of u and *learning coefficients* (λ_u, θ_u) such that for all smaller nbhds U,

$$\int_U e^{-Nf(\omega)}\,\varphi(\omega)d\omega \;\approx\; CN^{-\lambda_u}(\log N)^{\theta_u - 1}.$$

- *Sparsity penalty for MLE*: Given the log likelihood

$$\ell(u) = -\sum_{i=1}^{N} \log p(X_i|u),$$

for large samples we have the asymptotic approximation

$$-\log Z(u) \;\approx\; \operatorname{argmin}_{u\in\Omega}\, \ell(u) + \pi(u)$$

where $\pi(u) = \lambda_u \log N - (\theta_u - 1)\log\log N$.

- This is a generalization of the BIC to singular models.

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Integral Asymptotics

Faithfulness

- The *partial correlation (PC) algorithm* constructs directed Gaussian graphical models by inferring conditional independence statements $i \perp\!\!\!\perp j \mid S$ from the data.
- A distribution $p(\cdot|\omega)$ is *t-strong-faithful* to a graph G if

$$|\mathrm{corr}_{i,j|S}(\omega)| \leq t \;\Leftrightarrow\; i \text{ is } d\text{-separated from } j \text{ given } S.$$

- Using singular learning theory, we can approximate the volume of unfaithful parameters as t goes to zero.

$$\int_{|f(\omega)|\leq t} d\omega \;\approx\; Ct^{\lambda}(-\log t)^{\theta-1}$$

Here (λ, θ) is the learning coefficient of $f(\omega) = \mathrm{corr}_{i,j|S}(\omega)$. Determines performance of the PC algorithm for large samples.

- e.g. $(\lambda, \theta) = \begin{cases} (1,1) & \text{for all star trees,} \\ (1, p-1) & \text{for a chain with } p \text{ nodes.} \end{cases}$

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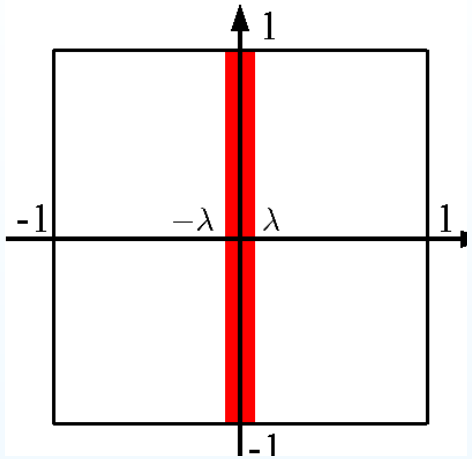
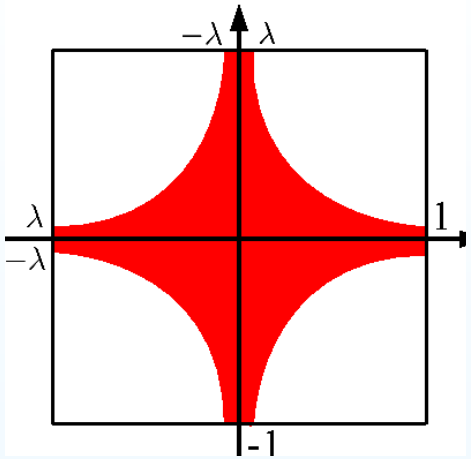
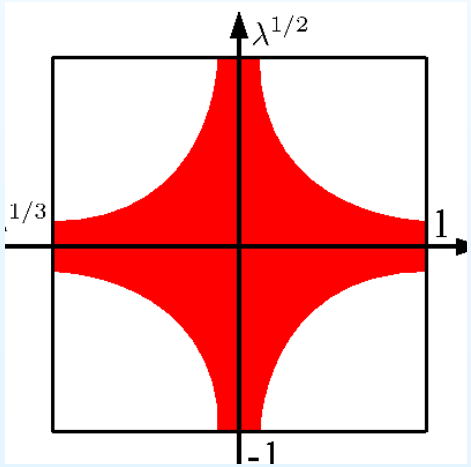
Faithfulness



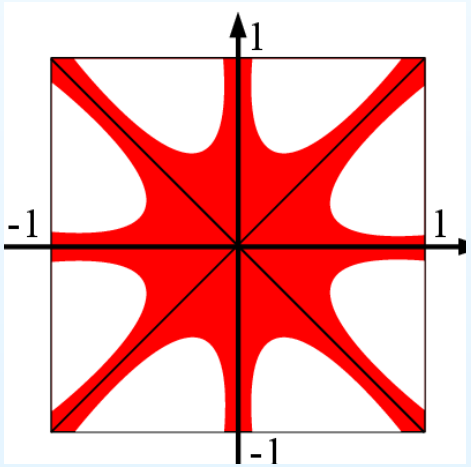
(a) x



(b) xy



(c) x^2y^3



(d) $x^3y - xy^3$

Tubes $|f(x,y)| \leq t$ for various polynomials in two variables.

Higher Order Asymptotics

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Integral Asymptotics

Higher order terms in the asymptotics of the integral can also be derived by resolving the singularities, generalizing the results of Shun and McCullagh (1995) for smooth models. For example,

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

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

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

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

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

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

Sparsity Penalties

Singular Learning

- Sumio Watanabe
- Bayesian Statistics
- Geometry
- Likelihood Ratio
- Integrated Likelihood

Integral Asymptotics

Singular Learning Theory

Sparsity Penalties

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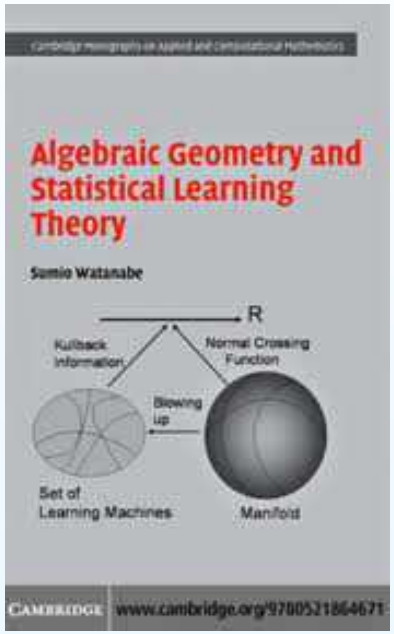
Integral Asymptotics

Sumio Watanabe

Sumio Watanabe



Heisuke Hironaka

In 1998, Sumio Watanabe discovered how to study the asymptotic behavior of singular models. His insight was to use a deep result in algebraic geometry known as *Hironaka's Resolution of Singularities*.

Heisuke Hironaka proved this celebrated result in 1964.
His accomplishment won him the Field's Medal in 1970.

Bayesian Statistics

X random variable with state space $\mathcal{X}$ (e.g. $\{1, 2, \ldots, k\}$, $\mathbb{R}^k$)
Δ space of probability distributions on $\mathcal{X}$

$\mathcal{M} \subset \Delta$ statistical model, image of $p : \Omega \to \Delta$
Ω parameter space
$p(x|\omega)dx$ distribution at $\omega \in \Omega$
$\varphi(\omega)d\omega$ prior distribution on Ω

Suppose samples $X_1, \ldots, X_N$ drawn from *true distribution* $q \in \mathcal{M}$.

Integrated likelihood $$Z_N = \int_\Omega \prod_{i=1}^N p(X_i|\omega)\, \varphi(\omega) d\omega.$$

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

Geometry of Singular Models

Sparsity Penalties

Singular Learning

- Sumio Watanabe
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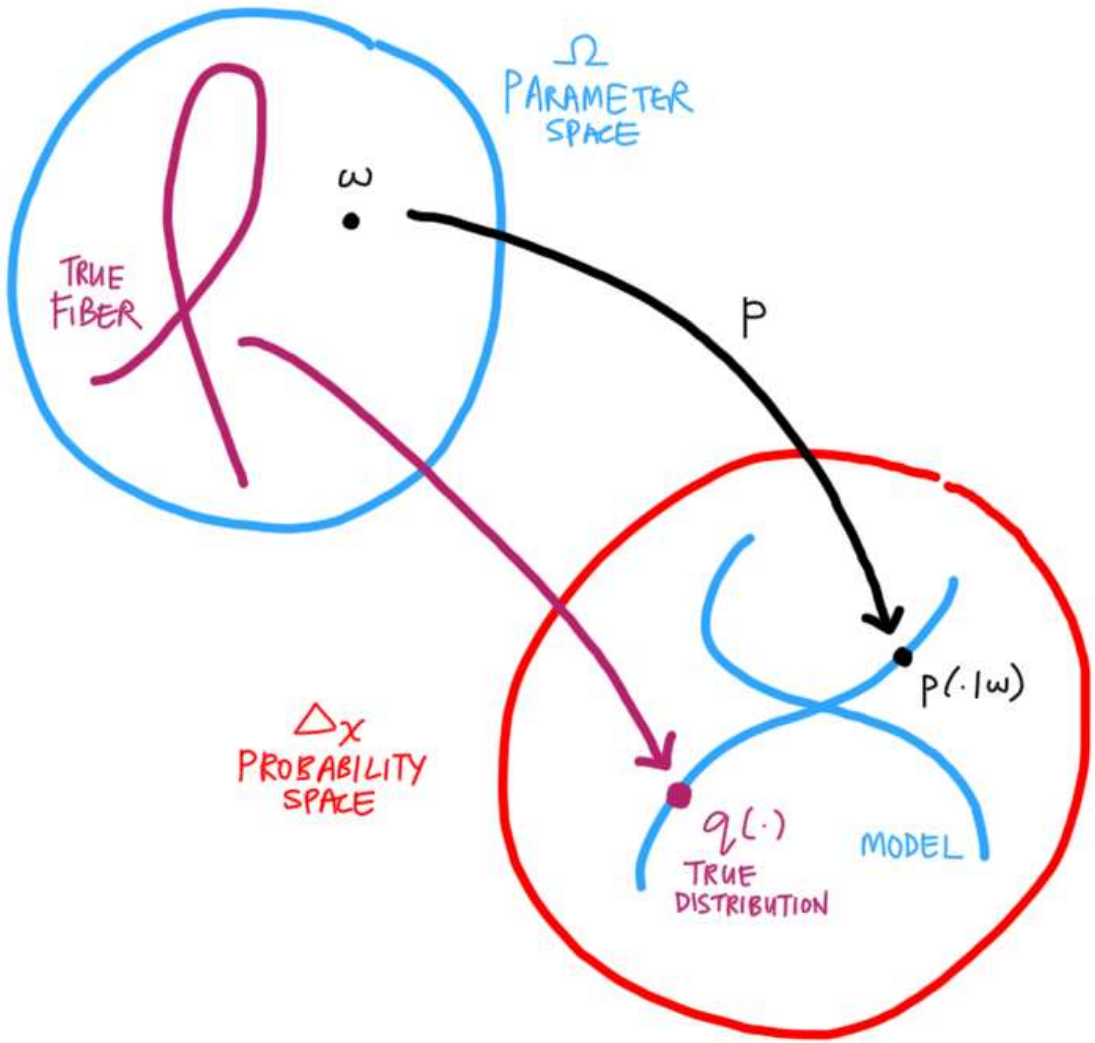
Integral Asymptotics



Standard Form of Log Likelihood Ratio

Define *log likelihood ratio*. Note that its expectation is $K(\omega)$.

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

Standard Form of Log Likelihood Ratio (Watanabe)

If $\rho : U \to \Omega$ desingularizes $K(\omega)$, then on each patch U_i,

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

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

For regular models, this is a *Central Limit Theorem*.

The integrated likelihood Z_N can be written in terms of K_N:

$$Z_N = \int_{\Omega} e^{-NK_N(\omega)}\varphi(\omega)d\omega$$

Asymptotics of Integrated Likelihood

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

Convergence of stochastic complexity (Watanabe)

The *stochastic complexity* has the asymptotic expansion

$$-\log Z_N = NS_N + \lambda_q \log N - (\theta_q - 1)\log\log N + O_p(1)$$

where λ_q, θ_q describe the asymptotics of the deterministic integral

$$Z(N) = \int_\Omega e^{-NK(\omega)}\varphi(\omega)d\omega \approx CN^{-\lambda_q}(\log N)^{\theta_q - 1}.$$

For regular models, this is the Bayesian Information Criterion.

Various names for (λ_q, θ_q):

statistics - *learning coefficient* of the model $\mathcal{M}$ at q

algebraic geometry - *real log canonical threshold* of $K(\omega)$

Sparsity Penalties

Singular Learning

Integral Asymptotics

- Estimation
- RLCT
- Geometry
- Desingularization
- Algorithm
- Open Problems

Integral Asymptotics

Estimating Integrals

Generally, there are three ways to estimate statistical integrals.

1. *Exact methods*
   Compute a closed form formula for the integral, e.g. Baldoni·Berline·De Loera·Köppe·Vergne, 2008; Lin·Sturmfels·Xu, 2009.

2. *Numerical methods*
   Approximate using Markov Chain Monte Carlo (MCMC) and other sampling techniques.

3. *Asymptotic methods*
   Analyze how the integral behaves for large samples.

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

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Real Log Canonical Threshold

Asymptotic theory (Arnol'd·Guseĭn-Zade·Varchenko, 1985) states that for a Laplace integral,

$$Z(N) = \int_{\Omega} e^{-Nf(\omega)} \varphi(\omega) d\omega \approx e^{-Nf^*} \cdot CN^{-\lambda} (\log N)^{\theta - 1}$$

asymptotically as $N \to \infty$ for some positive constants C, λ, θ and where $f^* = \min_{\omega \in \Omega} f(\omega)$.

The pair (λ, θ) is the *real log canonical threshold* of $f(\omega)$ with respect to the measure $\varphi(\omega) d\omega$.

Geometry of the Integral

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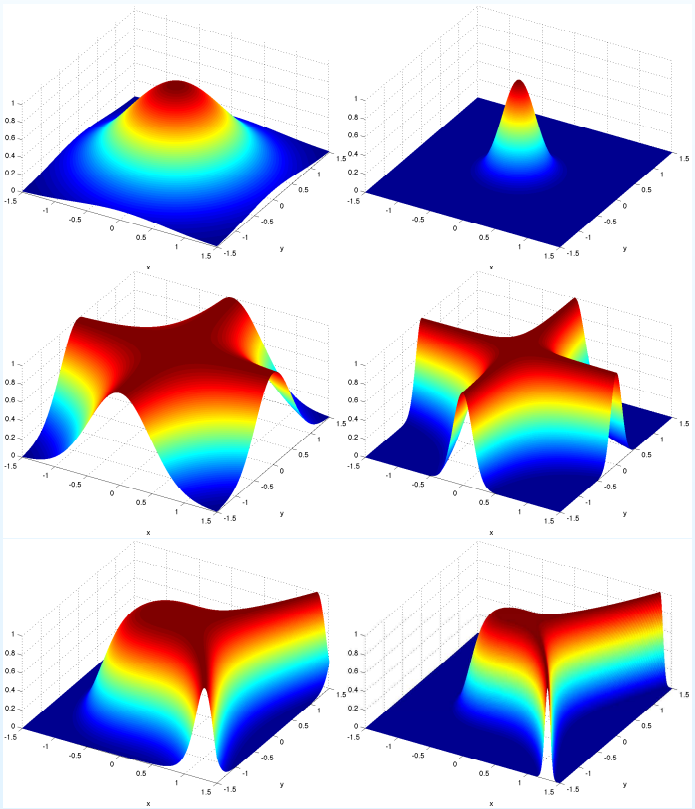
$$Z(N) = \int_\Omega e^{-Nf(\omega)}\varphi(\omega)d\omega \approx e^{-Nf^*} \cdot CN^{-\lambda}(\log N)^{\theta-1}$$

Integral asymptotics depend on *minimum locus* of exponent $f(\omega)$.

$$f(x,y) = x^2 + y^2$$
$$(\lambda, \theta) = (1, 1)$$

$$f(x,y) = (xy)^2$$
$$(\lambda, \theta) = (\tfrac{1}{2}, 2)$$

$$f(x,y) = (y^2 - x^3)^2$$
$$(\lambda, \theta) = (\tfrac{5}{12}, 1)$$



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

Desingularizations

Sparsity Penalties

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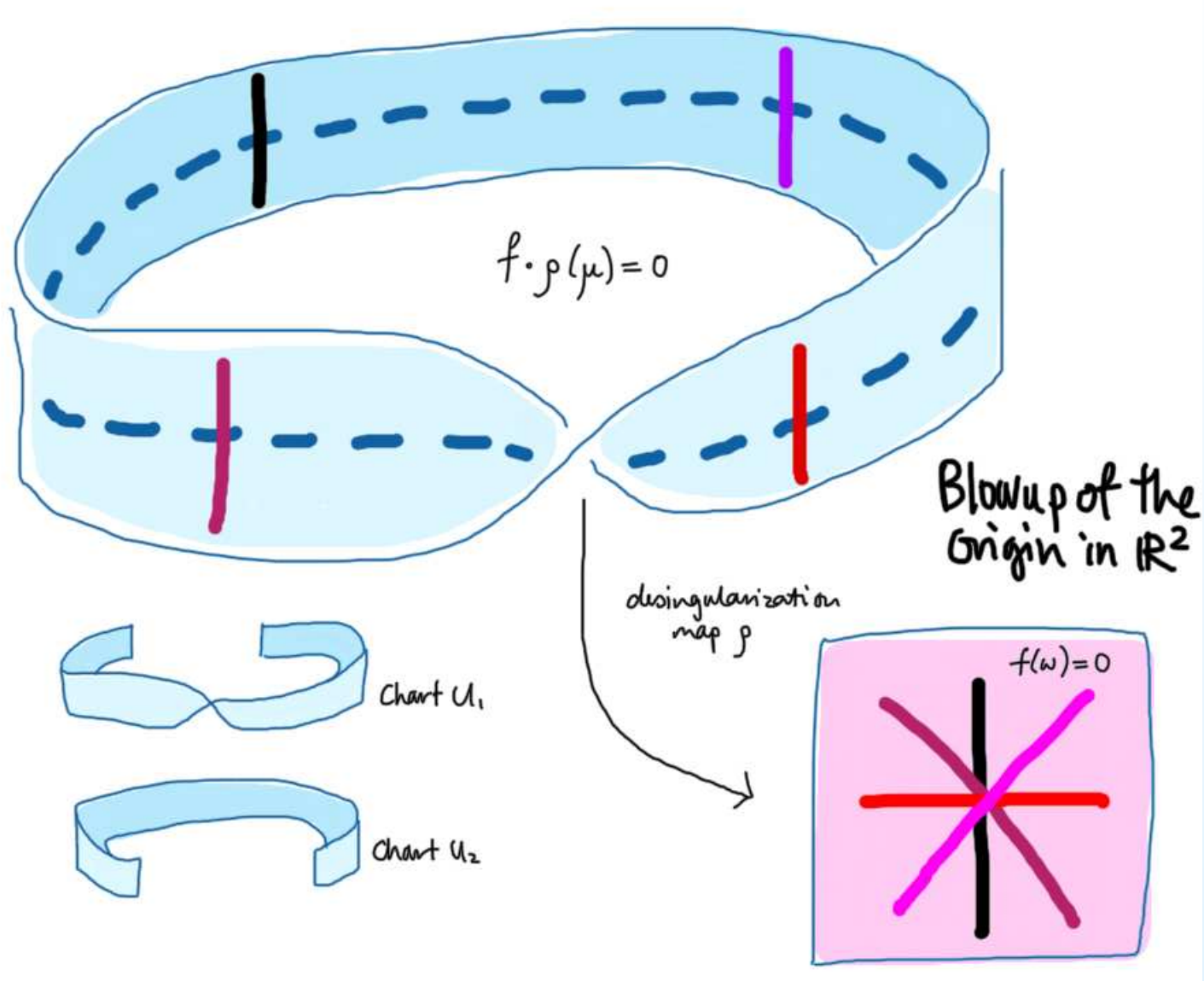

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Desingularizations

Let $\Omega \subset \mathbb{R}^d$ and $f : \Omega \to \mathbb{R}$ real analytic function.

- We say $\rho : U \to \Omega$ *desingularizes* f if

  1. U is a d-dimensional real analytic manifold covered by coordinate patches $U_1, \ldots, U_s$ ($\simeq$ subsets of $\mathbb{R}^d$).

  2. ρ is a proper real analytic map that is an isomorphism onto the subset $\{\omega \in \Omega : f(\omega) \neq 0\}$.

  3. For each restriction $\rho : U_i \to \Omega$,
  $$f \circ \rho(\mu) = a(\mu)\mu^{\kappa}, \quad \det \partial\rho(\mu) = b(\mu)\mu^{\tau}$$
  where $a(\mu)$ and $b(\mu)$ are nonzero on U_i.

- Hironaka (1964) proved that desingularizations always exist.

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Algorithm for Computing RLCTs

- We know how to find RLCTs of *monomial functions* (AGV, 1985).

$$\int_\Omega e^{-Na(\mu)\mu^\kappa} b(\mu)\mu^\tau d\mu \approx CN^{-\lambda}(\log N)^{\theta-1}$$

  where $\lambda = \min_i \frac{\tau_i+1}{\kappa_i}$, $\theta = |\{i : \frac{\tau_i+1}{\kappa_i} = \lambda\}|$.

- To compute the RLCT of any function $f(\omega)$:

  1. Find minimum f^* of f over Ω.
  2. Find a desingularization ρ for $f - f^*$.
  3. Use AGV Theorem to find (λ_i, θ_i) on each patch U_i.
  4. $\lambda = \min\{\lambda_i\}$, $\theta = \max\{\theta_i : \lambda_i = \lambda\}$.

- The difficult part is finding a desingularization, e.g (Bravo·Encinas·Villamayor, 2005).

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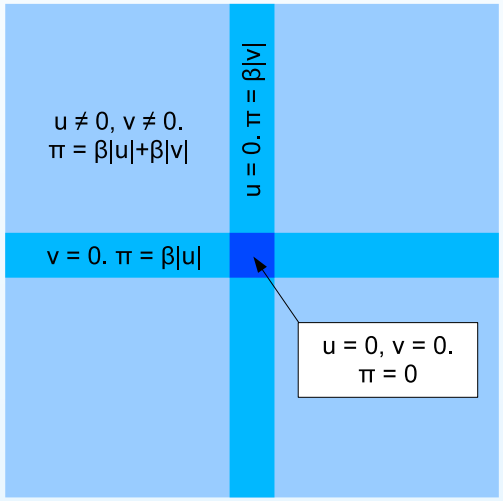
Open Problems

- How do we generalize LASSO to singular models?

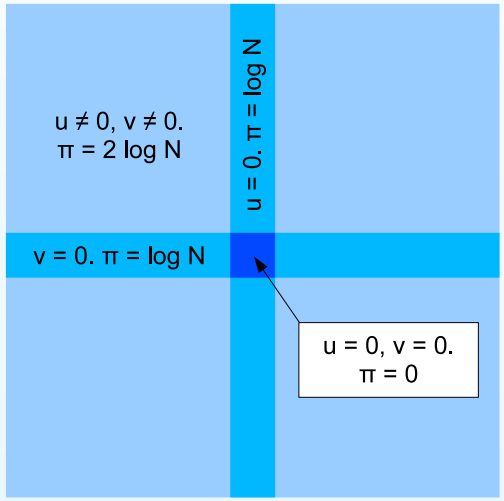
LASSO

$$\pi(\omega) = |\omega|_1 \cdot \beta$$



Bayesian Info Criterion (BIC)

$$\pi(\omega) = |\omega|_0 \cdot \log N$$



(Parameter space partitioned into regions with different weights.)

- How do we understand sparsity in any given statistical model? Occam's razor? Minimum message length? Shannon capacity?
- How do we use RLCTs to improve MCMC techniques?

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Thank you!

"Algebraic Methods for Evaluating Integrals in Bayesian Statistics"

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

(PhD dissertation, May 2011)

References

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