Understanding the Curse of Singularities in Machine Learning

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Sparsity Penalties

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	$\operatorname{argmin}_\omega \sum_{i=1}^N \lvert Y_i - \omega \cdot X_i \rvert^2$
Penalized MLE	$\operatorname{argmin}_\omega \sum_{i=1}^N \lvert Y_i - \omega \cdot X_i \rvert^2 + \pi(\omega)$

- Commonly used penalties

LASSO	$\pi(\omega) = \lvert\omega\rvert_1 \cdot \beta$
Bayesian Info Criterion (BIC)	$\pi(\omega) = \lvert\omega\rvert_0 \cdot \log N$
Akaike Info Criterion (AIC)	$\pi(\omega) = \lvert\omega\rvert_0 \cdot 2$

- Common applications
  - Parameter estimation
  - Model selection (e.g. which entries in ω are nonzero?)

Parameter Estimation

- *Parameter estimation is a form of model selection!*
- MLE: given true parameter $u \in \mathbb{R}^d$, likelihood of data is

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

- LASSO: put Laplacian prior on the parameter space.
  Given true parameter $u \in \mathbb{R}^d$, likelihood of data is

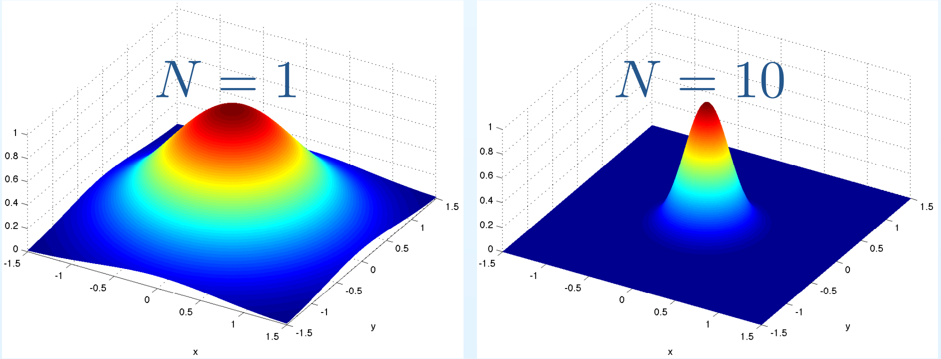
$$L(u) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}\sum_{i=1}^{N} |Y_i - u \cdot X_i|^2) \exp(-\frac{1}{2}\beta |u|_1)$$

- *Integrated likelihood*: put prior $\varphi(\omega)$ on small neighborhood Ω_u of true parameter $u \in \mathbb{R}^d$. Integrated likelihood of data is

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

Laplace Approximation

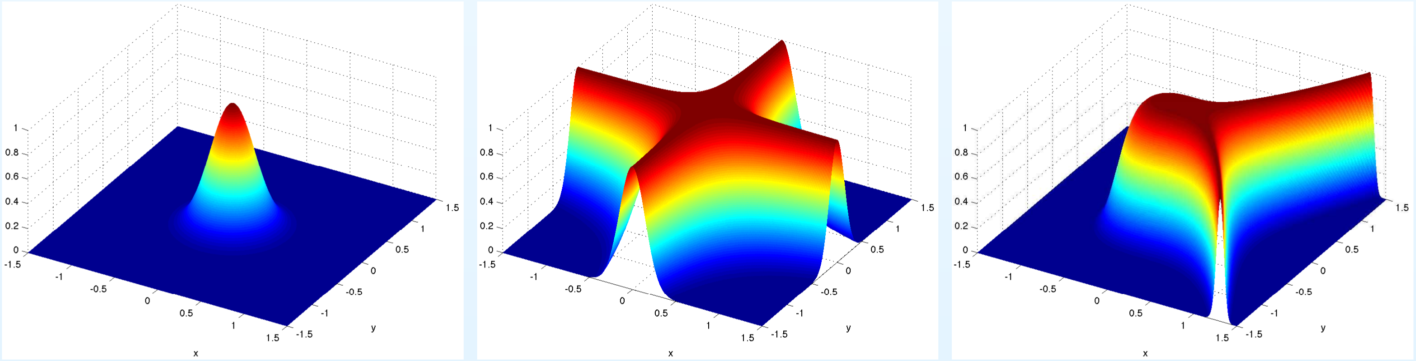
- Let $f(\omega) = \frac{1}{2N} \sum_{i=1}^{N} |Y_i - \omega \cdot X_i|^2$ so we can write
$$Z(u) = \frac{1}{\sqrt{2\pi}} \int_{\Omega_u} e^{-Nf(\omega)} \varphi(\omega) d\omega.$$
- *Laplace approximation*: If $f(\omega)$ is uniquely minimized at u and the Hessian satisfies $\det \partial^2 f(u) \neq 0$, 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.



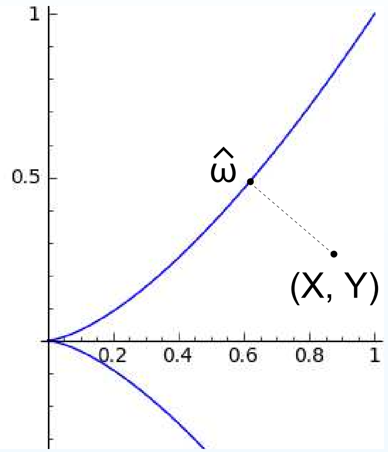
Graphs of $e^{-Nf(\omega)}$ for different N. Integral = Volume under graph.

Curse of Singularities

- The AIC, which is based on the *Bayes generalization error*, can also be derived using integral asymptotics.
- For *smooth* models i.e. $\det \partial^2 f(u) \neq 0$, 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?



Example: Singular Model



$$X \sim \mathcal{N}(\omega^2, 1), \quad Y \sim \mathcal{N}(\omega^3, 1)$$

data $(X_i, Y_i), i = 1 .. N$

parameter $\omega \in \mathbb{R}$, 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 $\pi(u) = \frac{1}{2} \log N$.

Higher Order 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,

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

$$\begin{aligned}
&\sqrt{\frac{\pi}{8}} N^{-\frac{1}{2}} \log N && -\sqrt{\frac{\pi}{8}} \left(\frac{1}{\log 2} - 2\log 2 - \gamma \right) N^{-\frac{1}{2}} \\
&-\frac{1}{4} N^{-1} \log N && +\frac{1}{4} \left(\frac{1}{\log 2} + 1 - \gamma \right) N^{-1} \\
&-\frac{\sqrt{2\pi}}{128} N^{-\frac{3}{2}} \log N && +\frac{\sqrt{2\pi}}{128} \left(\frac{1}{\log 2} - 2\log 2 - \frac{10}{3} - \gamma \right) N^{-\frac{3}{2}} \\
& && -\frac{1}{24} N^{-2} \quad + \cdots
\end{aligned}$$

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

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.

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

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

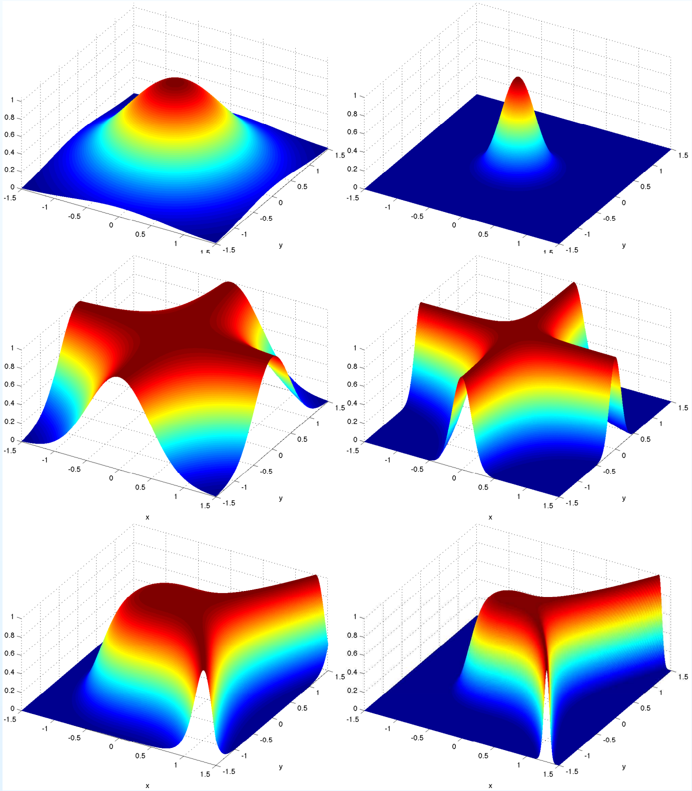
$$Z(N) = \int_\Omega e^{-Nf(\omega)}\varphi(\omega)d\omega \approx e^{-Nf^*} \cdot CN^{-\lambda}(\log N)^{\theta-1}$$

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

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

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

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



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

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

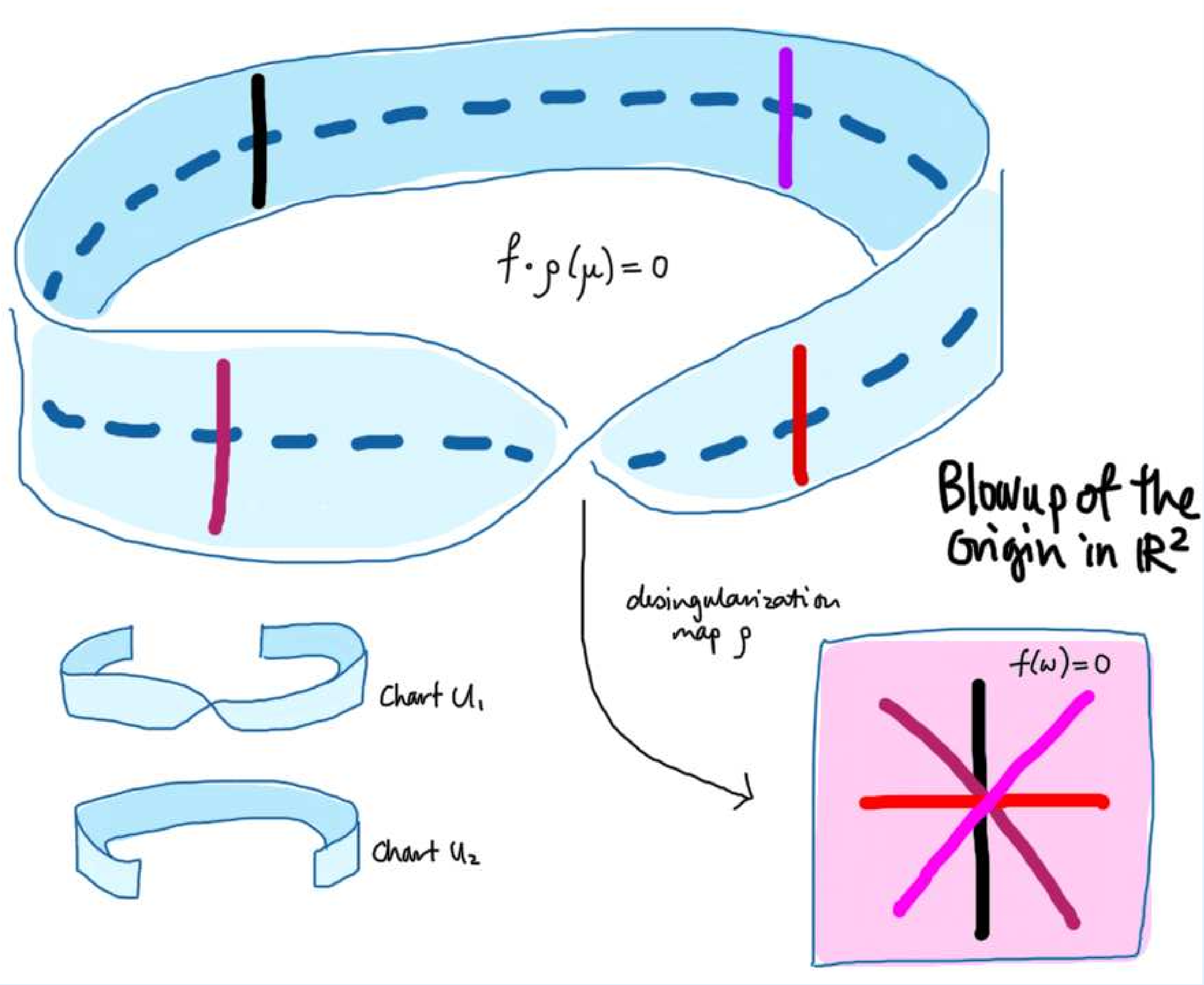
  1. U is a d-dimensional real analytic manifold covered by coordinate patches $U_1, \ldots, U_s$ ($\simeq$ subsets of $\mathbb{R}^d$).

  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.

Desingularizations



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

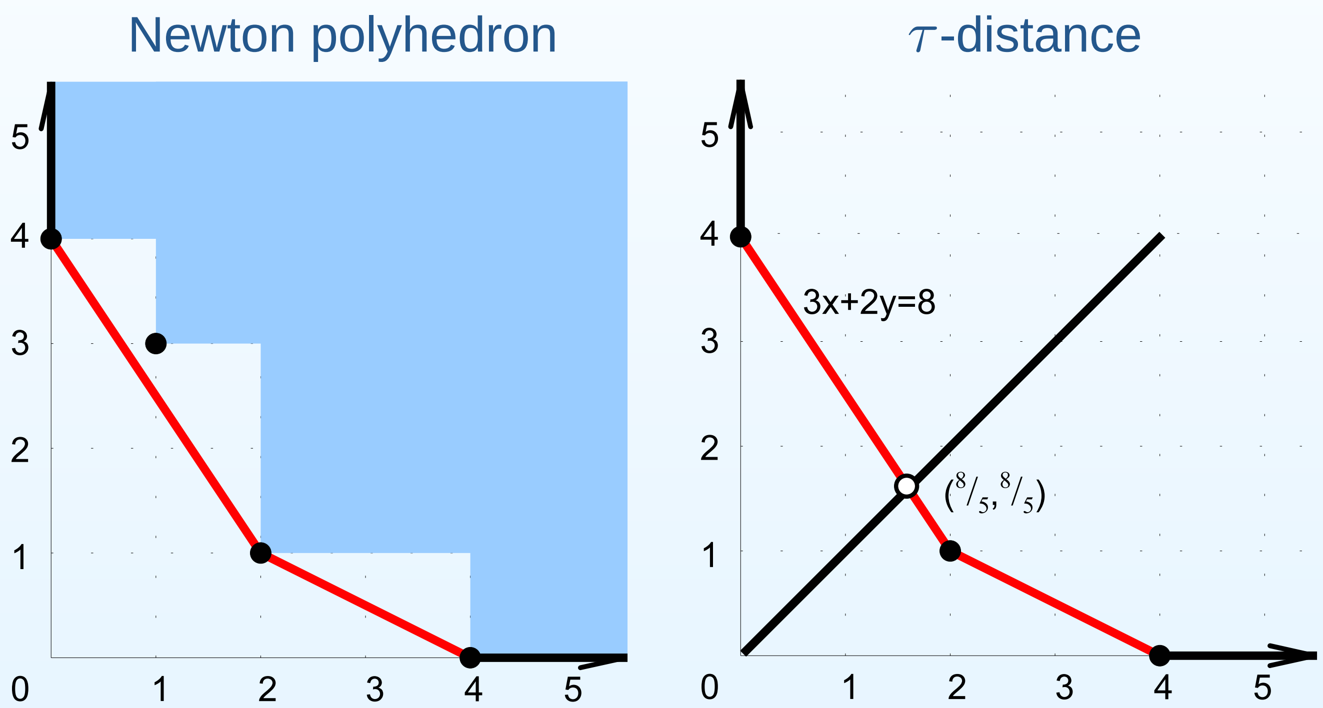
- To compute the RLCT of any function $f(\omega)$:
  1. Find minimum f^* of f over Ω.
  2. Find a desingularization ρ for $f - f^*$.
  3. Use AGV Theorem to find (λ_i, θ_i) on each patch U_i.
  4. $\lambda = \min\{\lambda_i\}$, $\theta = \max\{\theta_i : \lambda_i = \lambda\}$.

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

- One method for estimating RLCTs uses *Newton polyhedra*.

Newton Polyhedra

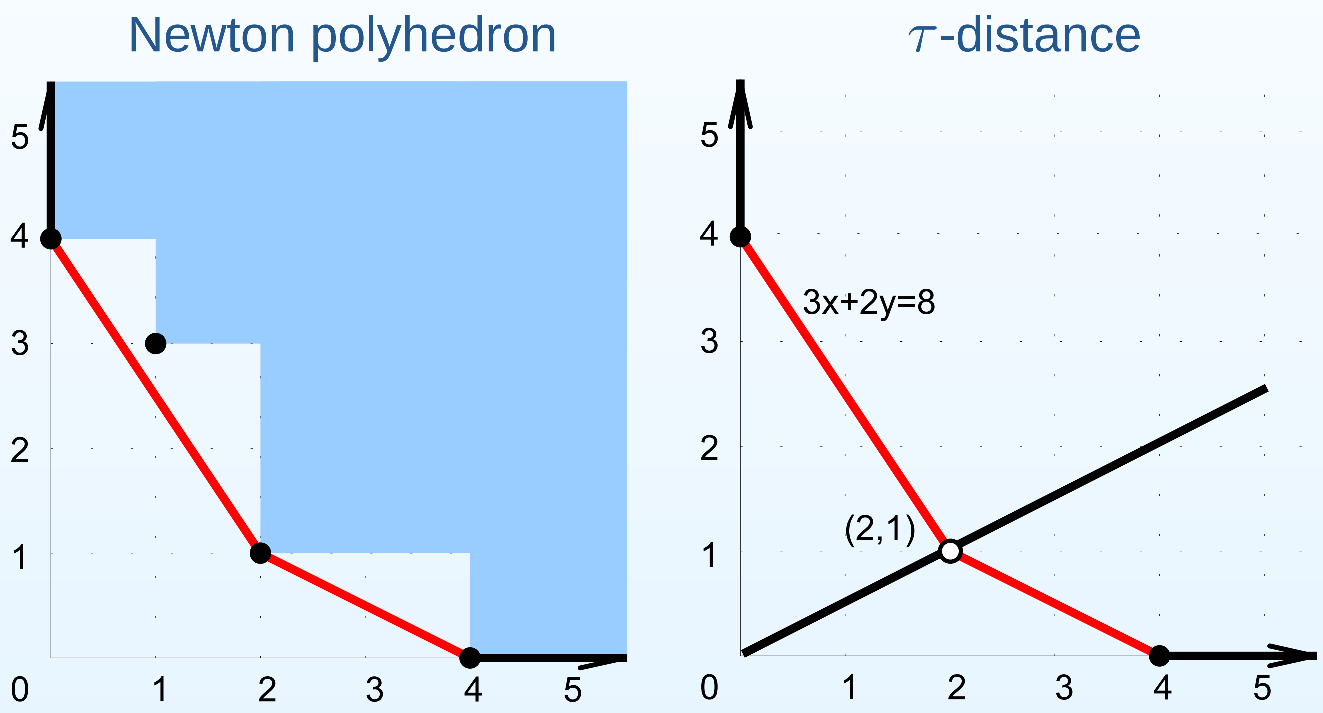
e.g. Let $f(x, y) = x^4 + x^2y + xy^3 + y^4$ and $\tau = (1, 1)$.



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

Newton Polyhedra

e.g. Let $f(x,y) = x^4 + x^2y + xy^3 + y^4$ and $\tau = (2,1)$.



The τ-distance is $l_\tau = 1$ and the multiplicity is $\theta_\tau = 2$.

Upper Bounds for RLCTs

Given a power series $f(\omega) \subset \mathbb{R}[\omega_1, \ldots, \omega_d]$,

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

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

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

1. *τ-distance* $l_\tau = \min\{t : t\tau \in \mathcal{P}(I)\}$.
2. *multiplicity* $\theta_\tau =$ codim of face of $\mathcal{P}(I)$ at this intersection.

Upper bound and equality for RLCTs at the origin

If l_τ is the τ-distance of $\mathcal{P}(f)$ and θ_τ is its multiplicity, then the RLCT (λ_0, θ_0) of f with respect to $\omega^{\tau-1}d\omega$ satisfies

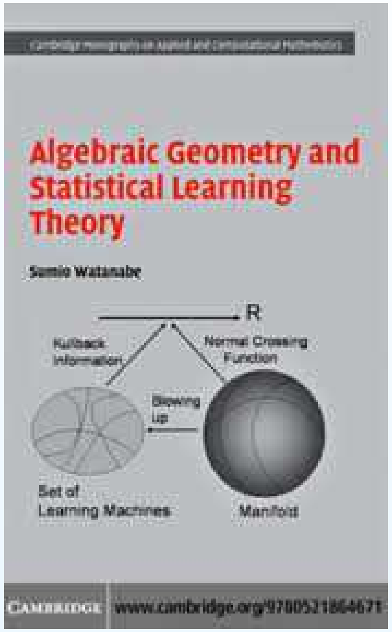
$$(\lambda_0, \theta_0) \leq (1/l_\tau, \theta_\tau).$$

Equality occurs when f is a *sum of squares of monomials*.

Singular Learning Theory

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 $\mathcal{X}$

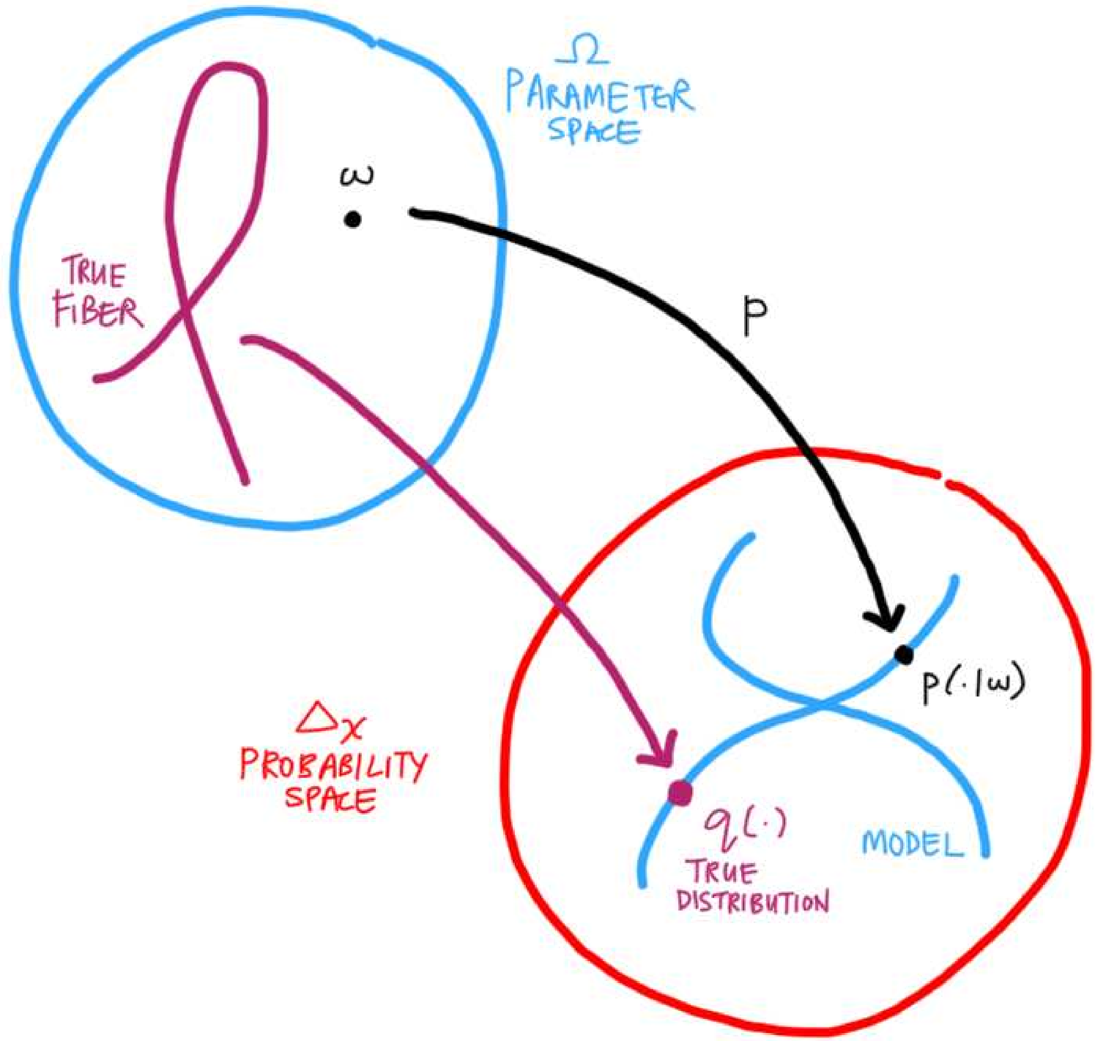
$\mathcal{M} \subset \Delta$	statistical model, image of $p : \Omega \to \Delta$
Ω	parameter space
$p(x\|\omega)dx$	distribution at $\omega \in \Omega$
$\varphi(\omega)d\omega$	prior distribution on Ω

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

Marginal 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



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*.

Learning Coefficient

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

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

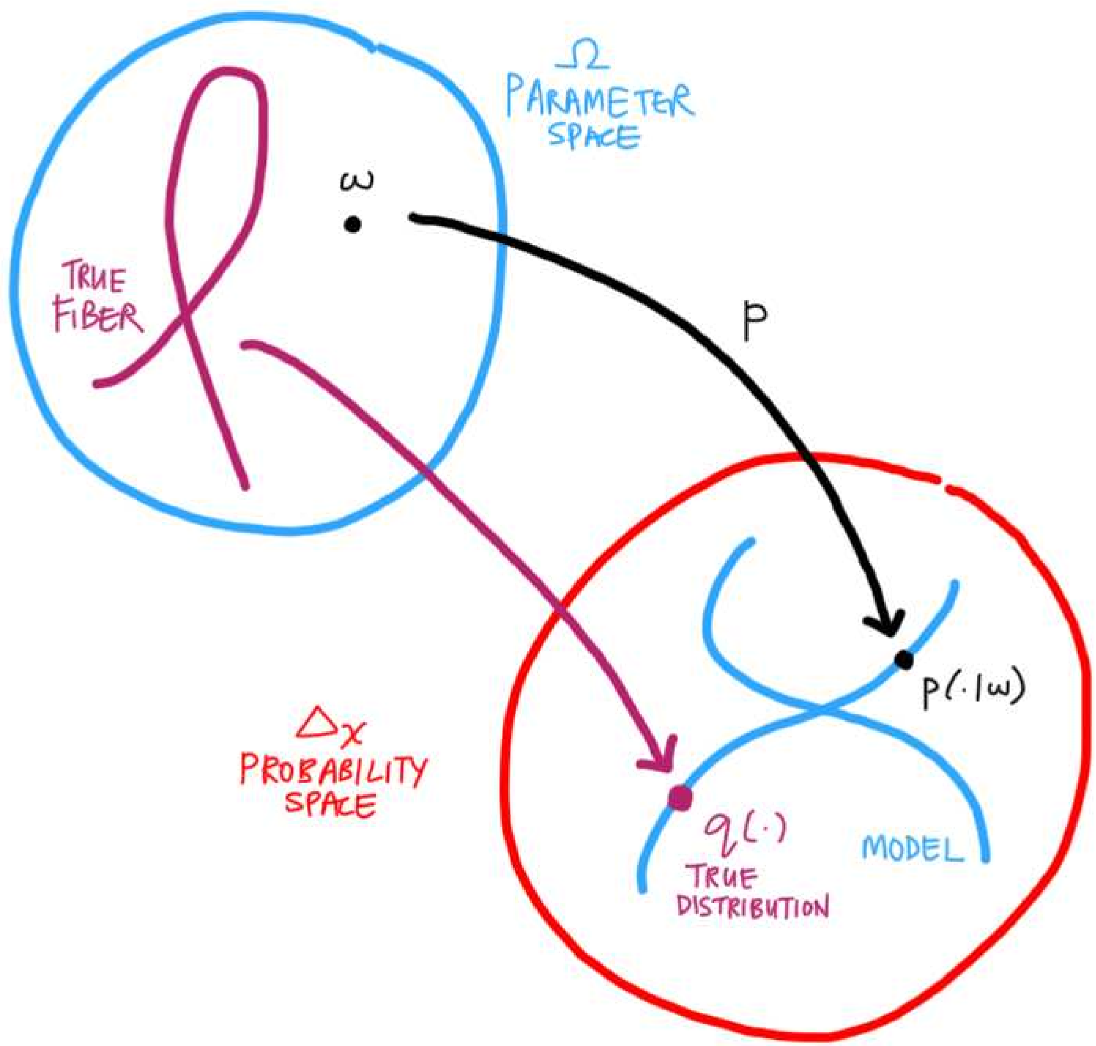
For regular models, this is the Bayesian Information Criterion.

Various names for (λ_q, θ_q):

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

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

Geometry of Singular Models



AIC and DIC

Bayes generalization error B_N. The Kullback-Leibler distance from the true distribution $q(x)$ to the predictive distribution $p(x|D)$.

Asymptotically, B_N is equivalent to

- Akaike Information Criterion for regular models

$$\text{AIC} = -\sum_{i=1}^{N} \log p(X_i|\omega^*) + d$$

- Akaike Information Criterion for singular models

$$\text{AIC} = -\sum_{i=1}^{N} \log p(X_i|\omega^*) + 2(\textit{singular fluctuation})$$

Numerically, B_N can be estimated using MCMC methods.

- Deviance Information Criterion for regular models

$$\text{DIC} \;=\; \mathbb{E}_X[\log p(X|\mathbb{E}_\omega[\omega])] - 2\,\mathbb{E}_\omega[\mathbb{E}_X[\log p(X|\omega)]]$$

- Widely Applicable Information Criterion for singular models

$$\text{WAIC} \;=\; \mathbb{E}_X[\log \mathbb{E}_\omega[p(X|\omega)]] - 2\,\mathbb{E}_\omega[\mathbb{E}_X[\log p(X|\omega)]]$$

Sparsity Penalty

- *Local RLCTs*: given $u \in \Omega$, there exist a small nbhd Ω_u of u and exponents (λ_u, θ_u) such that for all smaller nbhds U,

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

- *Maximum likelihood estimation*: $\mathrm{argmin}_{u \in \Omega}\, \ell(u)$ where

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

- *Sparsity penalty for MLE*: $\mathrm{argmin}_{u \in \Omega}\, \ell(u) + \pi(u)$ where

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

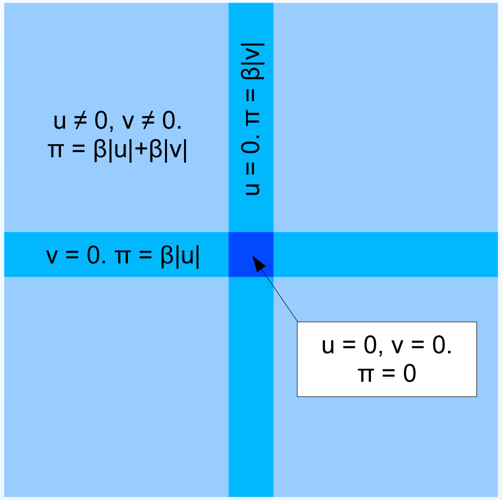
- This is a generalization of the BIC to singular models.

Open Problems

- How do we generalize LASSO to singular models?

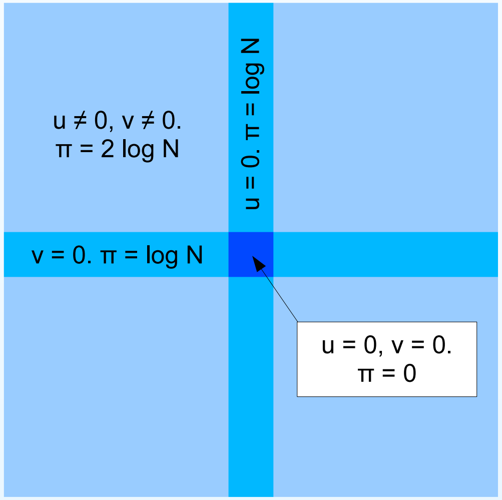
LASSO

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



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?

Thank you!

"Algebraic Methods for Evaluating Integrals in Bayesian Statistics"

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

(PhD dissertation, May 2011)

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