Recent Advances in Algebraic Geometry and Bayesian Statistics

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Abstract

This article is a review of theoretical advances in the research field of algebraic geometry and Bayesian statistics in the last two decades.

Many statistical models and learning machines which contain hierarchical structures or latent variables are called nonidentifiable, because the map from a parameter to a statistical model is not one-to-one. In nonidentifiable models, both the likelihood function and the posterior distribution have singularities in general, hence it was difficult to analyze their statistical properties. However, from the end of the 20th century, new theory and methodology based on algebraic geometry have been established which enables us to investigate such models and machines in the real world.

In this article, the following results in recent advances are reported. First, we explain the framework of Bayesian statistics and introduce a new perspective from the birational geometry. Second, two mathematical solutions are derived based on algebraic geometry. An appropriate parameter space can be found by a resolution map, which makes the posterior distribution be normal crossing and the log likelihood ratio function be well-defined. Third, three applications to statistics are introduced. The posterior distribution is represented by the renormalized form, the asymptotic free energy is derived, and the universal formula among the generalization loss, the cross validation, and the information criterion is established.
Two mathematical solutions and three applications to statistics based on algebraic geometry reported in this article are now being used in many practical fields in data science and artificial intelligence.

1 Introduction

Many statistical models and learning machines which have hierarchical structure or latent variables are widely used in data science, artificial intelligence, bioinformatics, economics, political science, psychology, and so on. Such models and machines are called nonidentifiable, since the map from a parameter to a probability density function is not one-to-one [44]. They are also called singular, because both the likelihood function and the posterior distribution contain singularities which cannot be approximated by any Gaussian function. In fact, the Fisher information matrix contains zero eigen values and the Laplace approximation does not capture the essential property of the posterior distribution. In other words, the classical statistical theory which needs the regularity condition does not hold, resulting that hypothesis test, model selection, hyperparameter optimization, and learning by gradient decent should be studied from new perspective [20, 19, 51, 14, 8].

Such nonidentifiable and singular models and machines are not special but ubiquitous in modern statistics and machine learning. For example, neural networks and deep learning [43, 44, 8] have hierarchical structures, normal mixtures [60, 24], Poisson mixtures [35], multinomial mixtures [58], and latent Dirichlet allocations [22] have latent or hidden variables, and matrix factorizations [6, 21], Boltzmann machines [62, 7], and Markov models [61, 67] have both hidden and hierarchical parts. In other words, almost all statistical models and learning machines which extract hidden structures or hierarchical inferences are nonidentifiable and singular [47].

Here let us illustrate the two mathematical problems which are universally found in nonidentifiable and singular models and machines. Let \( X \) and \( X_1, X_2, ..., X_n \) be independently and identically distributed \( \mathbb{R}^N \)-valued random variables and let \( h(x, \theta) \) be a real-valued function on \( \mathbb{R}^N \times \mathbb{R}^d \) which is analytic for \( \theta \) and satisfies \( H(\theta) = \mathbb{E}[h(X, \theta)] \geq 0 \). In statistics and machine learning, a random process \( H_n(\theta) \) defined on \( \mathbb{R}^d \),

\[
H_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} h(X_i, \theta)
\]

is quite often studied, in fact, the minus log density ratio function is a typical example. It can be rewritten as

\[
nH_n(\theta) = nH(\theta) - (nH(\theta))^{1/2} A_n(\theta),
\]
where \( A_n(\theta) \) is defined by

\[
A_n(\theta) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left\{ \frac{H(\theta) - h(X_i, \theta)}{H(\theta)^{1/2}} \right\}.
\]

Note that \( E[A_n(\theta)] = 0 \) for any \( \theta \) by the definition. If \( H(\theta) = 0 \) at a unique parameter \( \theta_0 \) and the Hessian matrix of \( H(\theta) \) at \( \theta_0 \) is positive definite, then regular statistical theory holds, resulting that the learning curves are determined by the dimension of the parameter \([1, 5, 29]\). However, if otherwise, there are two mathematical difficulties.

The first mathematical problem in singular statistics is that the set defined by \( H(\theta) = 0 \) consists of not a single element but multiple and uncountable elements with singularities. Hence the function \( H(\theta) \) cannot be approximated by any quadratic form in neighborhoods of \( H(\theta) = 0 \), moreover, it is difficult to measure the volume of \( \{ \theta : H(\theta) < t \} \) for \( t \to +0 \) near singularities although it determines the accuracy of Bayesian statistics.

The second problem is that the random process \( A_n(\theta) \) is not well-defined on \( H(\theta) = 0 \). In the region \( H(\theta) > 0 \), \( A_n(\theta) \) is an empirical process which converges to a Guassian process in distribution as \( n \) tends to infinity. However, \( H(\theta) - h(x, \theta) \) is not divisible by \( H(\theta)^{1/2} \) in general, hence in a neighborhood of \( H(\theta) \to +0 \), the limit process \( A_n(\theta) \to 0/0 \) cannot be determined uniquely.

In this paper, we show that algebraic geometry gives a mathematically natural solution to the foregoing statistically essential problems. Assume that \( H(\theta) \) is an arbitrary analytic function. Then, based on the resolution theorem which was proved by Hironaka \([23]\) and applied by Atiyah and Kashiwara \([9, 26]\), there exists an appropriate analytic function from a manifold to the parameter space,

\[
\theta = g(u),
\]

such that \( H(g(u)) \) is normal crossing on an arbitrary neighborhood of \( H(g(u)) = 0 \). Here a function \( H(g(u)) \) is said to be normal crossing if \( H(g(u)) \) is represented by a simple direct product of \((u_j)^{k_j}\), whose mathematical definition is given in Section 3. This theorem enables us to study the function \( H_n(\theta) \) and solves two mathematical problems. First, we can derive that the volume of the set \( \{ w : H(w) < t \} \) as \( t \to +0 \) is in proportion to \( t^{\lambda}(-\log t)^{m-1} \), where \( \lambda \) and \( m \) are birational invariants called a real log canonical threshold and a multiplicity. We show that the accuracy of Bayesian statistics is determined by this volume. Second, also we show that \( A_n(g(u)) \) is made to be a well-defined function of \( u \) because \( H(g(u)) - h(x, g(u)) \) is divisible by \( H(g(u))^{1/2} \), hence the empirical process theory ensures that \( A_n(g(u)) \) converges to a
Gaussian process on $u$ in distribution even in an arbitrary neighborhood of $H(g(u)) = 0$.

These two solutions have three applications to statistics. First, the posterior distribution is represented by the renormalized form, which clarifies the scaling law of the posterior distribution. Second, the asymptotic free energy, which is equal to the minus log marginal likelihood, is derived. Lastly, the universal formula among the generalization loss, the cross validation, and the information criterion is proved, by which the generalization loss for unknown information source can be estimated.

This article consists of six chapters. In Section 2, we explain the framework of Bayesian statistics and introduce two important random variables, the free energy and the generalization loss, which are measures of appropriateness of a statistical model and a prior distribution. In Section 3 mathematical description of Hironaka resolution theorem is introduced, by which we can represent the average log density ratio function can be made normal crossing, and two birational invariants, the real log canonical threshold and its multiplicity are defined. In Sections 4 and 5, two mathematical solutions and three applications to statistics are explained. Lastly, in Section 6 the results of this paper is summarized.

2 Framework of Bayesian Statistics

In this section, we prepare a mathematical framework of Bayesian statistics and explain the purpose of this paper.

Let $p(x|\theta)$ be a conditional probability density function of $x \in \mathbb{R}^N$ for a given parameter $\theta \in \Theta \subset \mathbb{R}^d$ and $\pi(\theta)$ be a probability density function of $\theta$. In Bayesian statistics, a candidate pair made by a person

$$\theta \sim \pi(\theta), \tag{1}$$

$$X^n \sim \prod_{i=1}^n p(x_i|\theta), \tag{2}$$

is investigated, which means $X^n = \{X_1, X_2, ..., X_n\}$ may be subject to a statistical model $p(x|\theta)$ with a prior distribution $\pi(\theta)$.

If $X_1, X_2, ..., X_n, ...$, are assumed to be subject to some distributions such as eqs. (1) and (2), they are called exchangeable. If they are exchangeable,
by de Finetti’s theorem, there exist both $Q(q)$ and $q(x)$ such that
\begin{align}
q(x) & \sim Q(q), \\
X^n & \sim \prod_{i=1}^n q(x_i),
\end{align}
where $Q(q)$ is a probability distribution on the set of all probability distributions on $\mathbb{R}^N$ and $q(x)$ is a probability density function which is subject to $Q(q)$. The general pair $Q(q)$ and $q(x)$ contains a specific pair $\pi(\theta)$ and $p(x|\theta)$, hence if a person makes a candidate pair $\pi(\theta)$ and $p(x|\theta)$ and rejects the existence of unknown $Q(q)$ and $q(x)$, it is a mathematical contradiction.

In statistical science of a large world, both $Q(q)$ and $q(x)$ are unknown and all models are wrong. A person cannot believe in a specific pair of a statistical model and a prior distribution because it is under- or over-parametrized in an environment of unknown uncertainty. In other words, a person who made $p(x|\theta)$ and $\pi(\theta)$ is aware that both are only fictional candidates, resulting that it is necessary to check or evaluate its appropriateness from a mathematically general viewpoint.

In this paper, we explain a role of algebraic geometry in modern Bayesian statistics. It is assumed that $X^n$ and $X$ are independent and generated from the unknown data-generating process $q(x)$ which is subject to $Q(q)$ and that a candidate pair, $p(x|\theta)$ and $\pi(\theta)$, is prepared by a person. Let $\mathbb{E}[f(X^n)|q]$ and $\mathbb{E}_X[f(X)|q]$ denote the expectation values of given functions $f(X^n)$ and $f(X)$ according to $\prod_i q(x_i)$ and $q(x)$, respectively.

The average and empirical log loss functions $L(\theta)$ and $L_n(\theta)$ are defined by
\begin{align}
L(\theta) &= -\mathbb{E}_X[\log p(X|\theta)|q], \\
L_n(\theta) &= -\frac{1}{n} \sum_{i=1}^n \log p(X_i|\theta).
\end{align}

The posterior distribution and the posterior predictive distribution using a
The candidate pair eqs. (1) and (2) are defined respectively by

\[ p(\theta|X^n) = \frac{1}{p(X^n)} \pi(\theta) \prod_{i=1}^{n} p(X_i|\theta), \]

\[ p(x|X^n) = \int p(x|\theta)p(\theta|X^n)d\theta, \]

where

\[ p(X^n) = \int \pi(\theta) \prod_{i=1}^{n} p(X_i|\theta)d\theta \]

is the marginal likelihood. The average and variance by using the posterior distribution \( p(\theta|X^n) \) are denoted by \( \mathbb{E}_\theta[\ ] \) and \( \mathbb{V}_\theta[\ ] \) respectively.

The free energy \( F_n \), which is equal to the minus log marginal likelihood, and the generalization loss \( G_n \) are defined respectively by

\[ F_n = -\log p(X^n), \]

\[ G_n = -\mathbb{E}_X[\log p(X|X^n)|q]. \]

Then it follows that

\[ \mathbb{E}[F_n|q] = \text{KL}(q(X^n)||p(X^n)) + nS(q), \]

\[ \mathbb{E}[G_n|q] = \text{KL}(q(X)||p(X|X^n)) + S(q), \]

where \( \text{KL}(\ || \ ) \) is Kullback-Leibler divergence of \( q_1(x) \) and \( q_2(x) \),

\[ \text{KL}(q_1(X)||q_2(X)) = \int q_1(x) \log \frac{q_1(x)}{q_2(x)} dx, \]

and \( S(q) \) is the entropy of \( q(x) \),

\[ S(q) = -\int q(x) \log q(x) dx. \]

Note that \( S(q) \) does not depend on the candidate pair \( p(x|\theta) \) and \( \pi(\theta) \). Therefore, the average free energy and the average generalization loss are minimized if and only if \( q(X^n) = p(X^n) \) and \( q(x) = p(x|X^n) \), respectively. These properties show that the free energy and the generalization loss can be understood as different measures of appropriateness of the pair \( p(x|\theta) \) and \( \pi(\theta) \). By the definition, for an arbitrary positive integer \( n \),

\[ \mathbb{E}[G_n|q] = \mathbb{E}[F_{n+1}|q] - \mathbb{E}[F_n|q] \]
holds, however, the pair \((p(x|\theta), \pi(\theta))\) that minimizes \(F_n\) is different from the pair that minimizes \(G_n\) [57].

Minimizing the free energy, which is equivalent to maximizing the marginal likelihood, is often employed in Bayesian model selection and hyperparameter optimization [2]. It is also known that the difference of the free energies between the null hypothesis pair and the alternative pair gives the most powerful Bayesian test [24]. Also minimizing the generalization loss is often adopted for the purpose of the accurate prediction in statistics and machine learning [11, 49]. Hence it is important to clarify the mathematical properties of the free energy and the generalization loss.

In order to estimate the generalization loss, three random variables are defined, the training loss \(T_n\), the leave-one-out cross validation \(C_n\) [15, 38, 18], and the widely applicable information criterion \(W_n\) [49] respectively by

\[
T_n = \frac{1}{n} \sum_{i=1}^{n} \log p(X_i|X^n), \tag{13}
\]

\[
C_n = \frac{1}{n} \sum_{i=1}^{n} \log p(X_i|X^n \setminus X_i), \tag{14}
\]

\[
W_n = T_n + \frac{1}{n} \sum_{i=1}^{n} \nabla_\theta \log p(X_i|\theta), \tag{15}
\]

where \(X^n \setminus X_i\) is the set leaving \(X_i\) out from \(X^n\). We define a function \(\Omega(\theta)\) on \(\Theta\) by

\[
\Omega(\theta) \equiv \pi(\theta) \prod_{i=1}^{n} p(X_i|\theta). \tag{16}
\]

Then the posterior distribution is represented by

\[
p(\theta|X^n) = \frac{\Omega(\theta)}{\int \Omega(\theta')d\theta'},
\]

and the free energy is given by

\[
F_n = -\log \int \Omega(\theta)d\theta. \tag{17}
\]

The posterior average \(E_\theta[ \ ]\) and the posterior variance \(\nabla_\theta[ \ ]\) are also repre-
sented by $\Omega(\theta)$, hence
\begin{align}
G_n &= -\mathbb{E}_X[\log \mathbb{E}_\theta[p(X|\theta)]|q], \\
T_n &= -\frac{1}{n} \sum_{i=1}^{n} \log \mathbb{E}_\theta[p(X_i|\theta)], \\
C_n &= \frac{1}{n} \sum_{i=1}^{n} \log \mathbb{E}_\theta[1/p(X_i|\theta)], \\
W_n &= T_n + \frac{1}{n} \sum_{i=1}^{n} \log \nabla_{\theta} \log p(X_i|\theta),
\end{align}
are all represented by using $\Omega(\theta)$. If a statistical model contains hierarchical structure or latent variables, then $\Omega(\theta)$ cannot be approximated by any Gaussian function in general, because a statistical model may be under- or over-parametrized. The main purpose of this paper is to clarify what mathematical structure determines $\Omega(\theta)$, the posterior distribution, and the five random variables.

**Purpose of this paper.** In this paper, we characterize the integration $\Omega(\theta)d\theta$ from the algebro-geometric point of view, and derive the probabilistic behaviors of five random variables, the free energy $F_n$, the generalization loss $G_n$, the training loss $T_n$, the leave-one-out cross validation $C_n$, and the widely applicable information criterion $W_n$, even if $\Omega(\theta)$ is far from any Gaussian function.

In this paper, we mainly study the accuracy of the free energy and the posterior predictive distribution. Their performance for the case when the probabilities distributions are different between training and test are clarified \[63\] and the accuracy of the estimation of the latent variables are also derived by \[65\]. In Bayesian statistics, it is one of the most important researches how to approximate the posterior distribution using Markov chain Monte Carlo (MCMC). Although the purpose of this paper is not studying MCMC methods, an algebro-geometric study of the posterior distribution may be useful in the design of MCMC process in singular models and machines. For example, the optimal sequence of the inverse temperatures in exchange Monte Carlo are clarified by the property of singular posterior distributions \[30\].
3 Algebro-Geometric Foundation

In this section, we introduce an algebro-geometric foundation on which mathematical and statistical theory is constructed.

For simplicity, we assume \( \Theta \subset \mathbb{R}^d \) is a compact set whose open kernel is not empty and \( L(\theta) \) is an analytic function of \( \theta \) in some open set which contains \( \Theta \). The set of all parameters that make \( L(\theta) \) minimum is

\[
\Theta_0 = \{ \theta \in \Theta ; L(\theta) \text{ is minimum} \}.
\]

If there exists \( \theta_0 \in \Theta_0 \) such that \( q(x) = p(x|\theta_0) \), then \( q(x) \) is said to be realizable by \( p(x|\theta) \), or if otherwise it is said unrealizable. If \( \Theta_0 \) consists of a single element \( \theta_0 \) and if the Hessian matrix \( \nabla^2 L(\theta_0) \) is positive definite, then \( q(x) \) is said to be regular for \( p(x|\theta) \), or if otherwise it is said to be singular.

The set \( \Theta_0 \) is called an analytic set because it is the set of all zero points of an analytic function \( L(\theta) - L(\theta_0) \). If \( L(\theta) \) is a polynomial function, then it is called an algebraic set. We assume that \( p(x|\theta_0) \) does not depend on the choice of \( \theta_0 \in \Theta \). If \( q(x) \) is realizable by or regular for \( p(x|\theta) \), then such a condition is satisfied \([52]\). For the case when \( p(x|\theta_0) \) depends on \( \theta_0 \in \Theta_0 \), see \([31, 50]\).

A log density ratio function \( f(x, \theta) \) is defined by

\[
f(x, \theta) = \log(p(x|\theta_0)/p(x|\theta)),
\]

which is equivalent to

\[
p(x|\theta) = p(x|\theta_0) \exp(-f(x, \theta)).
\]

We define \( K(\theta) \) and \( K_n(\theta) \) by

\[
K(\theta) = \mathbb{E}_X[f(X, \theta)|q], \quad (23)
\]

\[
K_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} f(X_i, \theta). \quad (24)
\]

Then \( K(\theta) \) is a nonnegative function by the definition and

\[
L(\theta) = L(\theta_0) + K(\theta), \quad (25)
\]

\[
L_n(\theta) = L_n(\theta_0) + K_n(\theta), \quad (26)
\]

resulting that

\[
\frac{\Omega(\theta)}{\exp(-nL_n(\theta_0))} = \exp(-nK_n(\theta)). \quad (27)
\]
The set of all optimal parameters is equal to the set of all zero points of an analytic function $K(\theta)$,

$$\Theta_0 = \{ \theta : K(\theta) = 0 \},$$

which contains singularities in general. It has been difficult to study statistics and machine learning on the original parameter space because of singularities. The following theorem is the algebro-geometric foundation on which universal statistical theory can be constructed.

**Hironaka Resolution Theorem** [23, 9, 26]. There exist both a compact subset $M$ of a $d$-dimensional analytic manifold and a proper analytic function from $M$ to $\Theta$

$$g : M \ni u \mapsto g(u) \in \Theta$$

such that, in each local coordinate of $M$, $K(g(u))$ is normal crossing,

$$K(g(u)) = u^{2k} \equiv u_1^{2k_1} u_2^{2k_2} \cdots u_d^{2k_d},$$

$$\pi(g(u)) |g'(u)| = b(u) |u^h| \equiv b(u) |u_1^{h_1} u_2^{h_2} \cdots u_d^{h_d}|,$$

where $k = (k_1, k_2, ..., k_d)$ and $h = (h_1, h_2, ..., h_d)$ are multi-indices of nonnegative integers, in which at least one $k_i$ is a positive integer. Here $b(u) > 0$ is a positive analytic function, and $|g'(u)|$ is the absolute value of the Jacobian determinant of $\theta = g(u)$. The correspondence between $\Theta \setminus \Theta_0$ and $g^{-1}(\Theta \setminus \Theta_0)$ is one-to-one in any neighborhood of $\Theta_0$. Note that a function $\theta = g(u)$ is called proper if the inverse image of a compact set is also compact.

This is the basic and most important theorem in algebraic geometry. There exists an algebraic algorithm by which both $M$ and $\theta = g(u)$ can be found by finite recursive blow-ups [23]. If Newton diagram of $K(\theta)$ is nondegenerate, they are found by a toric modification, which was applied to statistics and machine learning [64]. Even if $K(\theta)$ is not an analytic function, if $K(\theta) = K_1(\theta) K_2(\theta)$ where $K_1(\theta)$ is analytic and $K_2(\theta) > 0$, then the same theory can be derived in Bayesian statistics. For concrete examples of this theorem in statistics and machine learning, see [48].

Based on Hironaka resolution theorem, Bayesian statistics of a pair on $\Theta$

$$(p(x|\theta), \pi(\theta))$$

is equivalent to that of a pair on $M$

$$(p(x|g(u)), \pi(g(u)) |g'(u)|).$$

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It follows that
\[
\frac{\Omega(\theta)d\theta}{\exp(-nL_n(\theta_0))} = \exp(-nK_n(g(u)))b(u)|u^h|du.
\] (30)

Using the resolution theorem eqs. (28) and (29), the real log canonical threshold (RLCT) \( \lambda \) and multiplicity \( m \) are defined by
\[
\lambda = \min_{L.C.} \min_{1 \leq j \leq d} \left( \frac{h_j + 1}{2k_j} \right),
\] (31)
\[
m = \max_{L.C.} \# \left\{ j ; \frac{h_j + 1}{2k_j} = \lambda \right\},
\] (32)

where \( \min_{L.C.} \) and \( \max_{L.C.} \) show the minimum and maximum values over all local coordinates respectively. Here we define \( \left( \frac{h_j + 1}{2k_j} \right) = \infty \) for \( k_j = 0 \), and \( \# \) means the number of elements of a set. Hence \( 0 < \lambda < \infty \) and \( 1 \leq m \leq d \). Since \( \Theta \) is compact and \( w = g(u) \) is proper, the number of all local coordinates is finite and the integration over \( u \) is given by the finite sum of integrations of local coordinates. Without loss of generality, each local coordinate can be chosen as \([0,1]^d\) by the appropriate preparation of local parameter. For a given function \( K(\theta) \), there are infinitely many pairs \( \mathcal{M} \) and \( w = g(u) \) that give the resolution of singularities, however, neither RLCT nor its multiplicity depends on the choice of such pairs, in other words, they are birational invariants [48].

It is well known that the concept of the log canonical threshold plays an important role in higher dimensional algebraic geometry [27] and the real log canonical threshold is the same concept in the real algebraic geometry [34]. It was found in [42] that RLCT determines the accuracy of Bayesian statistics and machine learning. In many statistical models and learning machines, the common singularities often appear which is called Vandermonde type singularities [8]. A concrete method and application to statistics and machine learning are introduced in [48, 52].

RLCT is determined uniquely for a given pair \((K(\theta), \pi(\theta))\). There are several mathematical properties.

1. If \( q(x) \) is regular for \( p(x|\theta) \) and \( \pi(\theta_0) > 0 \), then \( \lambda = d/2 \), \( m = 1 \).

2. If there exists \( \theta_0 \in \Theta_0 \) such that \( \nabla^2 L(\theta_0) = 0 \) and \( \pi(\theta_0) > 0 \), then \( 0 < \lambda < d/2 \).

3. Note that Jeffreys’ prior is equal to zero at singularities, and if Jeffreys’ prior is employed in singular models, then \( \lambda \geq d/2 \).

4. Assume that \( \lambda_j \ (j = 1, 2) \) are RLCTs of \((K_j(\theta_j), \pi_j(\theta_j))\). Then
• RLCT of \((\sum_j K_j(\theta_j), \prod_j \pi_j(\theta_j))\) is equal to \((\sum_j \lambda_j)\).

• RLCT of \((\prod_j K_j(\theta_j), \prod_j \pi_j(\theta_j))\) is equal to \((\min_j \lambda_j)\).

5. Assume that \(\lambda_j (j = 1, 2)\) are RLCTs of \((K_j(\theta), \pi_j(\theta))\) and that \(K_1(\theta) \leq c_1 K_2(\theta)\) and \(\pi_1(\theta) \geq c_2 \pi_2(\theta)\) for some \(c_1, c_2 > 0\). Then \(\lambda_1 \leq \lambda_2\).

These properties are helpful to study RCLTs of statistical models and learning machines. In fact, RCLTs of important statistical models and learning machines were found by developing resolution procedures in neural networks [44, 8], normal mixtures [60], Poisson mixtures [35], multinomial mixtures [58], general and nonnegative matrix facorizations [6, 21], Boltzmann machines [62, 7], hidden and general Markov models [61, 67] and latent Dirichlet allocations [22]. Note that singularities in statistical models and learning machines make the free energy and the generalization losses smaller if Bayesian inferences are employed, hence almost all learning machines are singular [47] and that’s good [59]. In mixture models, a Dirichlet distribution is often chosen for a prior distribution of the mixture ratio. Then the posterior distribution has a phase transition according to the hyperparameter of Dirichlet distribution [52, 58]. In the different phases, RCLTs are different and the supports of asymptotic posterior distributions are different [52].

4 Two Mathematical Solutions

In this section, we show two mathematical problems in Bayesian statistics are solved based on resolution theorem.

4.1 Singular Schwartz Distribution

In this subsection, the first mathematical problem is solved on the resolution theorem. A method how to analyze the set \(\{\theta \in \Theta : K(\theta) < \epsilon\}\) as \(\epsilon \to +0\) is constructed even when an analytic set \(K(\theta) = 0\) contains singularities. The mathematical method explained in this subsection is based on the researches of singular Schwartz distribution by Gel’fand and Atiyah [9, 20].

By the definition of RLCT, without loss of generality, we can assume that

\[
u = (u_a, u_b) \in \mathbb{R}^m \times \mathbb{R}^{d-m},
\]

which satisfies

\[
\left(\frac{h_j + 1}{2k_j}\right) = \lambda \quad (1 \leq j \leq m),
\]

\[
\left(\frac{h_j + 1}{2k_j}\right) > \lambda \quad (m + 1 \leq j \leq d),
\]
where \( \lambda \) is RLCT. In other words, \( u_a \) is the part of \( u \) which gives \( \lambda \) with multiplicity \( m \) and \( u_b \) is the other part of \( u \) which does not. A multi-index \( \mu \in \mathbb{R}^{d-m} \) is defined by

\[
\mu = \{ \mu_j = -2\lambda k_j + h_j ; \ m + 1 \leq j \leq d \} \in \mathbb{R}^{d-m}.
\]

The zeta function \( \zeta(z) \) for \( z \in \mathbb{C} \) and the state density function \( v(t) \) for \( t \in \mathbb{R} \) are defined respectively by

\[
\zeta(z) = \int K(\theta)^z \pi(\theta) d\theta,
\]

\[
v(t) = \int \delta(t - K(\theta)) \pi(\theta) d\theta,
\]

(33)

where \( \zeta(z) \) in \( \Re(z) > -\lambda \) is well-defined by the integration over \( \theta \), which can be analytically continued to the unique meromorphic function on the entire complex plane \( \Re \). Then the zeta function is equal to the Mellin transform of the state density function,

\[
\zeta(z) = \int v(t) t^z dt,
\]

therefore, the state density function is equal to the inverse Mellin transform of the zeta function. By this correspondence, concrete calculation \( \Re \) shows that

\[
\frac{1}{(z + \lambda)^m} \leftrightarrow c_0 t^{\lambda-1}(-\log t)^{m-1},
\]

where \( c_0 \) is a constant. By using the resolution map \( \theta = g(u) \), the zeta function is equal to the finite sum of the integrations over \( u \in [0,1]^d \) in local coordinates,

\[
\zeta(z) = \sum_{L.C.} \int_{[0,1]^d} K(g(u))^z \pi(g(u)) |g'(u)| du
\]

\[
= \sum_{L.C.} \int_{[0,1]^d} u^{2kz} |u^h| b(u) du
\]

\[
= \sum_{L.C.} \int_{[0,1]^d} u^{2kz+h} b(0, u_b) du
\]

\[
+ \sum_{L.C.} \int_{[0,1]^d} u^{2kz+h} (b(u_a, u_b) - b(0, u_b)) du.
\]

(34)

Let the first and second terms of eq.(34) be \( \zeta_1(z) \) and \( \zeta_2(z) \) respectively. The largest pole of \( \zeta_1(z) \) is \( -\lambda \) with the order \( m \), and the largest pole of
\( \zeta_2(z) \) is smaller than \((-\lambda)\) or its order is larger than \(m\), because \(b(u_a, u_b) - b(0, u_b)\) is divisible by \(u_a\). By using the inverse Mellin transform, the following asymptotic expansion of the state density function as \( t \to +0 \) is derived \[48, 52\],

\[
\delta(t - u^{2k})|u^h|b(u)du = t^{\lambda-1}(- \log t)^{m-1}du^* + o(t^{\lambda-1}(- \log t)^{m-1}),
\]

where \(du^*\) is an integration,

\[
du^* = \frac{\delta(u_a)(u_b)^\mu b(u)}{2^m(m-1)! \prod_{j=1}^m k_j} du.
\]

The asymptotic expansion eq.\((35)\) will be employed in the Bayesian theory in the following sections. Moreover, \(\text{Vol}(\varepsilon)\), which is the volume of the set of almost optimal parameters measured by the prior distribution, is given by

\[
\text{Vol}(\varepsilon) = \int_{K(\theta) < \varepsilon} d\pi(\theta) = \int_0^\varepsilon dt \int \delta(t - K(\theta))\pi(\theta)d\theta,
\]

is given by

\[
\text{Vol}(\varepsilon) = \sum_{L.C.} \int_0^\varepsilon dt \int \delta(t - u^{2k})|u^h|b(u)du \\
\propto \varepsilon^\lambda(- \log \varepsilon)^{m-1} + \text{small order}.
\]

It follows that

\[
\lambda = \lim_{\varepsilon \to +0} \frac{\log \text{Vol}(\varepsilon)}{\log \varepsilon},
\]

which shows that RLCT can be understood as the generalized dimension of the set \(K(\theta) = 0\). As is shown in the following sections, RLCT determines the accuracy of Bayesian inference.

### 4.2 Empirical Process and Renormalized Posterior

In this subsection, the second mathematical problem is solved on the resolution theorem. It has been difficult to treat the empirical process on the original parameter space in the neighborhood of singularities of \(K(\theta) = 0\).

The function \(K_n(\theta)\) in eq.\((24)\) is rewritten as

\[
K_n(\theta) = K(\theta) - \frac{1}{\sqrt{n}}K(\theta)^{1/2}\xi_n(\theta),
\]

14
where
\[ \xi_n(\theta) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left\{ \frac{K(\theta) - f(X_i, \theta)}{\sqrt{K(\theta)}} \right\} \]

which is not a well-defined function in general at \( K(\theta) = 0 \).

A function \( f(x, \theta) \) is said to have a relatively finite variance, if there exists a constant \( c_0 > 0 \) such that, for an arbitrary \( \theta \in \Theta \),
\[
\int q(x)f(x, \theta)^2dx \leq c_0 K(\theta). \tag{38}
\]

Since \( \Theta \) is a compact set, this inequality holds in \( K(\theta) > 0 \). If \( q(x) \) is regular for \( p(x|\theta) \), then \( K(\theta) \) is a positive definite quadratic among \( K(\theta) = 0 \). Hence, eq. (38) holds. If \( q(x) \) is realizable by \( p(x|\theta) \), then also eq. (38) holds. In this paper, we study the case when eq. (38) holds. When \( q(x) \) is unrealizable and singular for \( p(x|\theta) \), then eq. (38) does not hold in general, resulting that the free energy has the different behavior from this paper [30, 31].

Assume that \( f(x, \theta) \) has a relatively finite variance and that \( K(g(u)) = u^{2k} \) is normal crossing. Then by the factor theorem, for each \( u_j \), \( f(x, g(u))^2 \) is divisible by \( u_j^{2k} \), hence \( f(x, g(u))^2 \) is divisible by \( K(g(u)) \). That is say, there exists a function \( a(x, u) \) which is analytic for \( u \) and
\[ f(x, g(u)) = a(x, u)u^k. \]

Then by the definition, \( \mathbb{E}_X[a(X, u)|q] = u^k \). It follows that \( \xi_n(u) \equiv \xi_n(g(u)) \) is given by
\[
\xi_n(u) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \{\mathbb{E}_X[a(X, u)|q] - a(X_i, u)\} = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \{u^k - a(X_i, u)\} \tag{39}
\]
is a well-defined function of \( u \) and
\[
K_n(g(u)) = u^{2k} - \frac{1}{\sqrt{n}} u^k \xi_n(u). \tag{41}
\]

Here \( \xi_n(u) \) is an empirical process which converges to a Gaussian process in distribution \( \xi_n(u) \to \xi(u) \) on each local coordinate \([0, 1]^d\). The Gaussian process \( \xi(u) \) is uniquely characterized by the conditions,
\[
\mathbb{E}[\xi_n(u)|q] = \mathbb{E}_{\xi}[\xi(u)] = 0, \tag{42}
\]
\[
\mathbb{E}[\xi_n(u)\xi_n(v)|q] = \mathbb{E}_{\xi}[\xi(u)\xi(v)] = \mathbb{E}_X[a(X, u)a(X, v)|q] - u^k v^k, \tag{43}
\]
where $E_{\xi}[\cdot]$ shows the expectation value over $\xi(u)$. Note that and $\xi(u)$ and $\xi_n(u)$ have the same expectation and covariance. Since the convergence of $\xi_n(u) \to \xi(u)$ is given by the uniform topology on $u \in \mathcal{M}$, it follows that
\[
\lim_{n \to \infty} E_u[|\xi_n(u)|^2] = E_{\xi}[|\xi(u)|^2]
\]
where $E_{\xi}[\cdot]$ means the average over Gaussian process $\xi(u)$.

**Standard Representation.** Let us summarize the two mathematical solutions in subsections 4.1 and 4.2. Even for nonidentifiable and singular statistical models and learning machines, there exists an appropriate representation of a parameter $\theta = g(u)$, such that the average and the log likelihood functions eq.(6) and eq.(5) can be rewritten as
\[
L(g(u)) = L(\theta_0) + u^{2k}, \quad (44)
\]
\[
L_n(g(u)) = L_n(\theta_0) + u^{2k} - \frac{1}{\sqrt{n}} u^k \xi_n(u), \quad (45)
\]
in each local coordinate of the manifold $\mathcal{M} = g^{-1}(\Theta)$. In other words, for an arbitrary triple $(q(x), p(x|\theta), \pi(\theta))$, universal properties of Bayesian statistics can be derived from the normal crossing representation eq.(45).

In this paper, we mainly study Bayesian statistics, however, the standard form eq.(45) can be applied to the maximum likelihood and maximum a posteriori methods [48]. For example, let $\hat{\theta}$ be the maximum likelihood estimator. If there exists an odd number in $k = (k_1, k_2, ..., k_d)$, then by the compactness of $\Theta$,
\[
L(\hat{\theta}) = L(\theta_0) + \frac{1}{2n} \sup_{g(u) \in \Theta_0} |\xi_n(u)|^2, \quad (46)
\]
\[
L_n(\hat{\theta}) = L_n(\theta_0) - \frac{1}{2n} \sup_{g(u) \in \Theta_0} |\xi_n(u)|^2, \quad (47)
\]
where $\sup$ shows the supremum value over all optimal parameters $\Theta_0$.

The function $L_n(\hat{\theta})$ is made smaller by the maximum likelihood method than by Bayesian method, however, the function $L(\hat{\theta})$ becomes larger. This is a reason why Bayesian inference is better than the maximum likelihood method in nonidentifiable or singular models.

### 5 Three Applications to Statistics

In this section, we show that two mathematical solutions in subsections 4.1 and 4.2 are useful in three applications to statistics. First, the the posterior
distribution is represented by a well-defined renormalized posterior distribution in subsection 5.1, second, the asymptotic behavior of the free energy and its estimating methods are derived in subsection 5.2, lastly, the universal formula among the generalization loss, the cross validation loss, and the information criterion are established in subsection 5.3.

5.1 Renormalized Posterior Distribution

First, the asymptotic behavior of the posterior distribution is represented by using the renormalized posterior distribution. By applying eqs. (35) and (45), we can derive the asymptotic behavior of singular posterior distribution.

\[
\Omega(\theta)d\theta = \exp(-nK_n(\theta))\pi(\theta)d\theta = \exp(-nu^{2k} + \sqrt{n} u^k\xi_n(u)b(u)|u^h| du
\]

\[
= \int dt \delta(t - nu^{2k}) \exp(-t + \sqrt{t}\xi_n(u))b(u)|u^h| du
\]

\[
= \frac{(\log n)^{\mathbb{L}C}(\xi(u))}{n^\lambda} \int dt t^{\mathbb{L}C}(\xi_n(u)) du^* + o_p\left(\frac{(\log n)^{\mathbb{L}C}(\xi(u))}{n^\lambda}\right).
\]

The renormalized posterior distribution is defined by its expectation value \(\langle F(t, u) \rangle\) of a given function \(F(t, u)\),

\[
\langle F(t, u) \rangle = \sum_{\mathbb{L}C.} \int du^* dt F(t, u) t^{\mathbb{L}C}(\xi_n(u)) \frac{(\log n)^{\mathbb{L}C}(\xi(u))}{n^\lambda}.
\]

Also \(\langle F(t, u) \rangle_\infty\) is defined by eq.(49) whose \(\xi_n(u)\) is replaced by \(\xi(u)\). Then the renormalized posterior distribution satisfies

\[
\lim_{n \to \infty} \mathbb{E}[\langle F(t, u) \rangle|q] = \mathbb{E}_\xi[\langle F(t, u) \rangle_\infty].
\]

By using the renormalized posterior distribution, the asymptotic behavior of the posterior distribution is derived as follows. By the relation \(f(x, g(u)) = a(x, u)u^k\) and \(t = nu^{2k}\), the correspondence between the posterior distribution and the renormalized posterior distribution is derived for \(\alpha \geq 0\),

\[
\mathbb{E}_\theta[f(x, \theta)^\alpha] = \frac{1}{n^{\alpha/2}}\langle (a(x, u)\sqrt{t})^\alpha \rangle + o_p(1/n^{\alpha/2}).
\]
This equation shows that the log density ratio function has the $(1/n^{1/2})$ order. Moreover, there exist two equations which hold by the renormalized posterior distribution. First, by using a partial integration over $t$, it follows that

$$
\langle t^\alpha \rangle = (\lambda + \alpha - 1)\langle t^{\alpha-1} \rangle + \frac{1}{2}\langle t^{\alpha-1/2} \xi_n(u) \rangle.
$$

(51)

Second, let us define two random variables $\langle \sqrt{t} \xi_n(u) \rangle$ and

$$
V(\xi_n) = E_x[\langle ta(X, u)^2 \rangle - \langle \sqrt{t}a(X, u) \rangle^2] | q.
$$

Then by using the partial integration over the functional space $\xi(u)$, it follows that

$$
E_\xi[\langle \sqrt{t} \xi(u) \rangle_\infty] = E_\xi[V(\xi)].
$$

By using these properties, the asymptotic values of expectations by the posterior distribution are represented by the renormalized posterior distributions.

### 5.2 Asymptotic Free Energy

Second, the asymptotic free energy, which is equal to the minus log marginal likelihood, is derived. By applying eq.(48) to eq.(17), it follows that

$$
F_n = nL_n(\theta_0) + \lambda \log n - (m - 1) \log \log n
+ \chi(\xi_n) + o(1),
$$

(52)

$$
E[F_n|q] = nL(\theta_0) + \lambda \log n - (m - 1) \log \log n
+ E_\xi[\chi(\xi)] + o(1),
$$

(53)

where $\chi(\xi_n)$ is defined by

$$
\chi(\xi_n) = -\log \left( \sum_{L.C.} \int dt \ t^{\alpha-1} \exp(-t + \sqrt{t} \xi_n(u))du^* \right),
$$

which converges to $\chi(\xi)$ in distribution.

In general, it needs heavy computational costs to calculate the free energy $F_n$, hence alternative methods are desired. The real log canonical threshold depends on not only a pair $p(x|\theta)$ and $\pi(\theta)$ but also an unknown probability distribution $q(x)$. Hence neither eqs. (52) nor (53) can be directly applied to numerical calculation of the free energy. Two methods were proposed for solving this problem for the case when the posterior distribution cannot be
approximated by any normal distribution. The first method was proposed by [12] that, by using the estimated RLCT \( \hat{\lambda} \), the singular BIC

\[
sBIC = nL_n(\hat{\theta}) + \hat{\lambda} \log n
\]

is defined, where \( \hat{\theta} \) is the maximum likelihood estimator. This is a generalized version of BIC [36] of regular statistical models to general singular models.

The second method [51] is as follows. We introduce a partition function for an inverse temperature \( \beta > 0 \),

\[
F(\beta) = -\log \int \prod_{i=1}^n p(X_i|\theta)^\beta \pi(\theta) d\theta
\]

Then \( F(0) = 0 \) and \( F(1) = F_n \), resulting that there exists \( 0 < \beta^* < 1 \) such that

\[
F_n = \frac{\int \prod_{i=1}^n p(X_i|\theta)^\beta \pi(\theta) d\theta}{\int \prod_{i=1}^n p(X_i|\theta)^\beta \pi(\theta) d\theta}
\]

(54)

(55)

Let the second term of the right hand side of eq.(55) be \( R_n \). Then by the same way as the renormalized posterior distribution is derived,

\[
R_n = \sum_{L.C.} \int du^* dt \left( t - \sqrt{t} \xi_n(u) \right) t^{\lambda-1} \exp(-\beta^* t + \beta^* \sqrt{t} \xi_n(u))
\]

\[
\sum_{L.C.} \int du^* dt t^{\lambda-1} \exp(-\beta^* t + \beta^* \sqrt{t} \xi_n(u))
\]

In this integration, by setting \( \beta^* = 1/\log n \) and by replacing \( t \) and \( dt \) by \( t/\beta^* \) and \( dt/\beta^* \) in the integration respectively, it follows that

\[
R_n = \lambda \log n + o_p(\log n).
\]

Therefore by the definition

\[
WBIC = F'(1/ \log n),
\]

we obtain

\[
WBIC = nL_n(\theta_0) + \lambda \log n + o_p(\log n).
\]

has the same asymptotic expansion as \( F_n \) according to the order \( \log n \). In the numerical calculation of WBIC, the posterior distribution with the inverse
temperature $1/\log n$ is necessary. An efficient algorithm to generate such posterior distribution in mixtures models are proposed \cite{54}.

In sBIC, no averaging calculation on the parameter set is required, but the theoretical results about RLCTs for several models are necessary. In WBIC, averaging on the parameter set is necessary, but the theoretical results about RLCTs are not required.

In the variational Bayes approaches, the Bayesian posterior distribution is approximated by an independent distribution $r(\theta) = r_1(\theta_1)r_2(\theta_2)$, and the variational free energy is defined as the minimization of the functional

$$F_{vb} = \inf_{r=r_1\cdot r_2} \left\{ -S(r) - \int r(\theta) \log \Omega(\theta) d\theta \right\},$$

where $S(r)$ is the entropy of $r(\theta)$ and $\inf$ is the infimum value overall probability distributions that are represented by $r(\theta) = r_1(\theta_1)r_2(\theta_2)$. In singular cases, the variational free energy has a different coefficient of the $\log n$ term from that of Bayesian free energy \cite{40, 66, 32, 25}. The Kullback-Leibler divergence between the posterior and approximated distributions is equal to the difference between the Bayes and variational free energies, hence the accuracy of the variational approximation is clarified by examining both free energies.

### 5.3 Generalization Loss and Its Estimators

Third, we show that the asymptotic behaviors of generalization loss and its estimators are clarified.

Let us introduce the functional cumulant generating functions \cite{49} for $\alpha \in \mathbb{R}$,

$$G(\alpha) = \mathbb{E} \log \mathbb{E}_d[p(X|\theta^\alpha)|q], \quad (56)$$

$$T(\alpha) = \frac{1}{n} \sum_{i=1}^{n} \log \mathbb{E}_d[p(X_i|\theta^\alpha)], \quad (57)$$

by which random variables $G_n$, $T_n$, $C_n$ and $W_n$ are represented,

$$G_n = -G(1), \quad (58)$$

$$T_n = -T(1), \quad (59)$$

$$C_n = T(-1), \quad (60)$$

$$W_n = -T(1) + T''(0). \quad (61)$$

20
Note that \( G(0) = T(0) = 0 \). It is shown in [49] that \( \mathbb{E}[G(\alpha)|q] = \mathbb{E}[T(\alpha)|q] \) and that, for \( k \geq 2 \),

\[
G^{(k)}(\alpha) = O_p(1/n^{k/2}), \quad \text{(62)}
\]

\[
T^{(k)}(\alpha) = O_p(1/n^{k/2}). \quad \text{(63)}
\]

The four random variables are represented by the functional cumulant generating functions,

\[
G_n = -G'(0) - \frac{1}{2}G''(0) + O_p(1/n^{3/2}), \quad \text{(64)}
\]

\[
T_n = -T'(0) - \frac{1}{2}T''(0) + O_p(1/n^{3/2}), \quad \text{(65)}
\]

\[
C_n = -T'(0) + \frac{1}{2}T''(0) + O_p(1/n^{3/2}), \quad \text{(66)}
\]

\[
W_n = -T'(0) + \frac{1}{2}T''(0) + O_p(1/n^{3/2}), \quad \text{(67)}
\]

By the definition of the log density ratio function eq.(22), it follows that

\[
-G'(0) = L(\theta_0) + \mathbb{E}_X[\mathbb{E}_\theta[f(X|\theta)]|q], \quad \text{(68)}
\]

\[
G''(0) = \mathbb{E}_X[\nabla^2_\theta[f(X|\theta)]|q], \quad \text{(69)}
\]

\[
-T'(0) = L_\theta(\theta_0) + \frac{1}{n} \sum_{i=1}^n \mathbb{E}_\theta[f(X_i|\theta)], \quad \text{(70)}
\]

\[
T''(0) = \frac{1}{n} \sum_{i=1}^n \nabla^2_\theta[f(X_i|\theta)]. \quad \text{(71)}
\]

By applying eq.(50) and eq.(51),

\[
G_n = L(\theta_0) + \frac{1}{n} \left( \lambda + \frac{1}{2} \langle \sqrt{t} \xi_n(u) \rangle - \frac{1}{2} V(\xi_n) \right) + o_p \left( \frac{1}{n} \right), \quad \text{(72)}
\]

\[
T_n = L_\theta(\theta_0) + \frac{1}{n} \left( \lambda - \frac{1}{2} \langle \sqrt{t} \xi_n(u) \rangle - \frac{1}{2} V(\xi_n) \right) + o_p \left( \frac{1}{n} \right), \quad \text{(73)}
\]

\[
C_n = L_\theta(\theta_0) + \frac{1}{n} \left( \lambda - \frac{1}{2} \langle \sqrt{t} \xi_n(u) \rangle + \frac{1}{2} V(\xi_n) \right) + o_p \left( \frac{1}{n} \right), \quad \text{(74)}
\]

\[
W_n = L_\theta(\theta_0) + \frac{1}{n} \left( \lambda - \frac{1}{2} \langle \sqrt{t} \xi_n(u) \rangle + \frac{1}{2} V(\xi_n) \right) + o_p \left( \frac{1}{n} \right). \quad \text{(75)}
\]
Let \( \nu = \mathbb{E}_\xi [V(\xi)]/2 \) be the *singular fluctuation*. It follows that

\[
\mathbb{E}[G_n|q] = L(\theta_0) + \frac{\lambda}{n} + o\left(\frac{1}{n}\right),
\]

(76)

\[
\mathbb{E}[T_n|q] = L(\theta_0) + \frac{\lambda - 2\nu}{n} + o\left(\frac{1}{n}\right),
\]

(77)

\[
\mathbb{E}[C_n|q] = L(\theta_0) + \frac{\lambda}{n} + o\left(\frac{1}{n}\right),
\]

(78)

\[
\mathbb{E}[W_n|q] = L(\theta_0) + \frac{\lambda}{n} + o\left(\frac{1}{n}\right).
\]

(79)

These results theoretically clarified the asymptotic behaviors of the generalization loss and its estimators, on which we can make Bayesian model evaluation methods. The leave-one-out cross validation (LOOCV) and WAIC can be employed even if \( q(x) \) is singular for \( p(x|w) \), whereas neither AIC [1] nor DIC [37]. When a leverage sample point is contained in a sample, the importance sampling cross validation eq.(20) becomes unstable [33, 13], and the difference between LOOCV and WAIC becomes larger [52, 55]. The improved version of numerical calculation of the cross validation was proposed in [39].

If a sample is independent, LOOCV and WAIC are equivalent to each other. However, if otherwise, they may not be equivalent. For example, in regression problems where the conditional probability distribution \( q(y|x) \) of an output \( Y \) for a given input \( X \), the input samples \( \{X_i\} \) may dependent or fixed and \( \{Y_i\} \) are conditionally independent. In such cases, LOOCV does not estimate the conditional generalization loss, whereas WAIC does [52, 55].

From eqs. (72), (73), (74), and (75), it is derived that the leave-one-out cross validation and the information criterion have the inverse correlation to the generalization loss, [49],

\[
(G_n - L(\theta_0)) + (C_n - L_n(\theta_0)) = \frac{2\lambda}{n} + o_p\left(\frac{1}{n}\right),
\]

(80)

\[
(G_n - L(\theta_0)) + (W_n - L_n(\theta_0)) = \frac{2\lambda}{n} + o_p\left(\frac{1}{n}\right).
\]

(81)

Although the cross validation and the information criterion are useful in many statistical applications, these properties clarified a disadvantages of them. Improved methods, adjusted cross validation and information criteria, combining leave-one-out and hold-out cross validations have been proposed [57], which make the variance of the estimators smaller.

From the viewpoint of the bias and variance problem, the effect of singularities are also studied. The probabilistic behaviors of the generalization
losses when the optimal parameter $\Theta_0$ is in a neighborhood of singularities were also clarified \[43\]. In singular models and machines, there are phase transitions as sample size increases \[46\].

6 Conclusion

We have reviewed recent advances in the research filed of algebraic geometry and Bayesian statistics. The two mathematical problems caused by singular log likelihood function were resolved by an algebro-geometric transform. There are two birational invariants which determine Bayesian statistics. The former is the real log canonical threshold which clarifies the singular dimension of a statistical model and a prior distribution. The latter is the singular fluctuation which indicates the functional variance of the log likelihood function. Based on the theoretical properties of these two concepts, three statistical problems were overcome. First, the posterior distribution was represented by a renormalized posterior distribution defined on a manifold. Second, the asymptotic behavior of the free energy was clarified and its estimation methods were constructed. Lastly, universal formulas between generalization loss, cross validation, and information criterion were derived. These mathematical and statistical results are now being used in data science and artificial intelligence.

Data Availability and Conflict of Interest

Data Availability

Data sharing is not applicable to this article as no data sets were generated or analyzed during the current study.

Conflict of interest

The corresponding author states that there is no conflict of interest.

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