Mathematical theory of Bayesian statistics for unknown information source

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In statistical inference, uncertainty is unknown and all models are wrong. That is to say, a person who makes a statistical model and a prior distribution is simultaneously aware that both are fictional candidates. To study such cases, statistical measures have been constructed, such as cross validation, information criteria and marginal likelihood; however, their mathematical properties have not yet been completely clarified when statistical models are under- or over-parametrized. We introduce a place of mathematical theory of Bayesian statistics for unknown uncertainty, which clarifies general properties of cross validation, information criteria and marginal likelihood, even if an unknown data-generating process is unrealizable by a model or even if the posterior distribution cannot be approximated by any normal distribution. Hence it gives a helpful standpoint for a person who cannot believe in any specific model and prior. This paper consists of three parts. The first is a new result, whereas the second and third are well-known previous results with new experiments. We show there exists a more precise estimator of the generalization loss than leave-one-out cross validation, there exists a more accurate approximation of marginal likelihood than Bayesian information criterion, and the optimal hyperparameters for generalization loss and marginal likelihood are different.

This article is part of the theme issue ‘Bayesian inference: challenges, perspectives, and prospects’.
1. Introduction

Bayesian inference is now widely employed in statistics and machine learning, because it provides a precise posterior predictive distribution when statistical models and learning machines have hierarchical structures or hidden variables. In fact, the more complex statistical models are necessary in practical applications, the more important Bayesian inference becomes. This is the reason why mathematical foundation of Bayesian statistics is necessary for the cases when models and machines are under- or over-parametrized, in other words, they are too simple or too complex to minimize the generalization loss.

In an older Bayesian statistics of the twentieth century, it was said that a person should have the ability to capture an uncertainty by a statistical model and to represent a degree of belief by a prior distribution. Also it was said that, if a model is made by synthesis of partial models, then the priors of partial models and their parameters should be determined. Nowadays, however, we know the set of all probability distributions is so large that a person cannot believe in any specific one even for personal decision, which is often referred to as ‘all models are wrong’ [1]. It was pointed out that a method how to determine or criticize a statistical model still remains unsolved [2]. In decision theory, coherent inference based on the subtle misspecification of a statistical model may take us to the wrong conclusion although it has been carefully prepared [3]. Hence, in Bayesian statistics, we need to check the posterior predictive distribution and improve a model as sample size increases, in other words, a statistical model that is fixed before observation of a sample is not optimal in general [4,5]. In the use of Bayesian statistics for a scientific purpose, preparation of a model and a prior needs rethinking outside of a small world [6]. A new paradigm was proposed that both a statistical model and a prior distribution are candidate systems that had better be optimized for an unknown data-generating process by mathematical procedures [7–9]. Based on these researches in the computer age [10], it was proposed that modern statistics is based on both computational algorithms and inferential evaluation, which has been accepted in statistics, data science and machine learning fields.

In this paper, we introduce a place of mathematical foundation of Bayesian statistics for the case when uncertainty is unknown in a large world. That is to say, we study a case when a person, who makes a pair of a statistical model and a prior distribution, is simultaneously aware that it is only a fictional candidate. Needless to say, there is no completely objective evaluation method, however, it is possible to prepare a much wider set of probability distributions that contain a person’s choice as a special one and to examine a candidate pair from a more generalized point of view.

Statistical evaluation measures for unknown data-generating process have been proposed, for example, cross validation, information criteria and marginal likelihood. However, their mathematical properties are not yet fully clarified, because, if a statistical model has hierarchical structure or latent variables, the posterior distribution is highly singular. In this paper, we clarify general theory when a statistical model is under- or over-parametrized, and show the following three mathematical properties. The first part is a new result, whereas the second and third parts are well-known previous results with new experiments.

First, although the leave-one-out (LOO) cross validation [11–13] and information criterion [14,15] have the same asymptotic expectation values as the generalization loss, it is clarified that they have inverse correlation to the generalization loss. Hence neither LOO cross validation nor information criterion is the best estimator of the generalization loss in general. In this paper, we show the better estimator can be made by using an adjusted cross validation that is a weighted sum of the LOO and the hold-out cross validations or the out-of-sample validation whose concrete definition is given in §3, equation (3.8).

Second, we study the asymptotic behaviour of the marginal likelihood when the posterior distribution is far from a normal distribution. If the posterior distribution can be approximated by some normal distribution, then the free energy, which is the minus log marginal likelihood, can be asymptotically approximated by Bayesian information criterion (BIC) [16] whose variance term is given by the half of dimension of the parameter space. We show that, if the posterior
distribution contains singularities, the half of the dimension of the parameter space in BIC is replaced by the real log canonical threshold whose definition is introduced in §2, equation (2.24). We also study several methods how to estimate the asymptotic free energy in such general cases.

Third, we compare the LOO cross validation, the widely applicable information criterion (WAIC) and the marginal likelihood as measures of a prior distribution.

When a candidate prior distribution is a parametric function of a hyperparameter, the optimal hyperparameter that minimizes the LOO cross validation or the WAIC converges to the optimal one that minimizes the average generalization loss, whereas the optimal hyperparameter that maximizes the marginal likelihood does not. Their equivalence and difference are studied theoretically and experimentally.

In §2, we explain a place of mathematical framework of the Bayesian statistics when uncertainty is unknown. Two statistical measures, the free energy and the generalization loss are defined when the data-generating process is unknown. Also the definition and meaning of the real log canonical threshold (RLCT) are introduced, which plays the central role in the theory of Bayesian statistics. In §3, we explain the probabilistic properties of the generalization loss, LOO cross validation and WAIC, and propose the more precise measure of the generalization loss can be made. In §4, the free energy or the minus log marginal likelihood is studied. In singular cases of overparametrized models, they cannot be approximated by BIC, but can by new algebraic geometrical studies. In §5, a prior optimization problem in a regular statistical model is analysed. In §§6 and 7, the results of this paper are discussed and concluded.

2. Mathematical framework of Bayesian statistics for unknown uncertainty

In this section, we introduce a mathematical framework of Bayesian statistics for a case when uncertainty is unknown.

Let $n$ be an arbitrary positive integer and $x^n = \{x_i \in \mathbb{R}^N, i = 1, 2, \ldots, n\}$ be a set of real vectors.

In this paper, we study a case when a statistical model is parametric and the set of parameters is a subset of a finite-dimensional Euclidean space. We assume that a person, an agent, or an artificial intelligence makes a candidate pair of a statistical model $p(x|\theta)$ and a prior distribution $\pi(\theta)$, where $\theta \in \Theta \subset \mathbb{R}^d$ is a parameter, such that

$$\theta \sim \pi(\theta)$$

and

$$x^n \sim \prod_{i=1}^n p(x_i|\theta).$$

Then the posterior and posterior predictive distributions based on equations (2.1) and (2.1) are automatically defined by

$$p(\theta|x^n) = \frac{1}{p(x^n)} \pi(\theta) \prod_{i=1}^n p(x_i|\theta)$$

and

$$p(x|x^n) = \int p(x|\theta)p(\theta|x^n) \, d\theta,$$

where $p(x^n)$ is the marginal likelihood,

$$p(x^n) = \int \pi(\theta) \prod_{i=1}^n p(x_i|\theta) \, d\theta.$$
Note. A sample $x^n$ is understood to be from a real world, whereas a pair $p(x|\theta)$ and $\pi(\theta)$ is a fictional candidate prepared by a person. Both $q(x)$ and $Q(q)$ may be interpreted as also abstract concepts in a person’s mathematical mind, or a scientific assumption of a data-generating process in the real world. It should be emphasized that the same mathematical theory holds, independently of the assumption that $q(x)$ and $Q(q)$ are real or unreal, because the mathematical framework is constructed for an arbitrary $p(x|\theta), \pi(\theta), q(x)$ and $Q(q)$. In both cases, if a pair $p(x|\theta)$ and $\pi(\theta)$ is provided, then the existence of $q(x)$ and $Q(q)$ is automatically derived. A person who cannot accept the existence of $q(x)$ or $Q(q)$ should also reject the candidate pair $p(x|\theta)$ and $\pi(\theta)$. For interpretation of the case studied in this paper, see §6a. In this paper, we mainly study exchangeable cases. For cases when a sample is neither independent nor exchangeable, see §6c.

For an arbitrary function $f(X^n)$ of $X^n$, its expectation value for $q(x)$ is defined by

$$\mathbb{E}[f(X^n)|q] = \int f(x^n) \prod_{i=1}^{n} q(x_i) \, dx_i.$$

The average and empirical entropies are respectively defined by

$$S(q) = -\int q(x) \log q(x) \, dx$$

and

$$S_n(q) = -\frac{1}{n} \sum_{i=1}^{n} \log q(x_i).$$

Two well-known functionals of $(p, \pi) \equiv (p(x|\theta), \pi(\theta))$, the free energy $F_n = F_n(p, \pi)$ and the generalization loss $G_n = G_n(p, \pi)$, which are the minus log marginal likelihood and the minus expected log likelihood, respectively, are defined by

$$F_n = -\log \int \pi(\theta) \prod_{i=1}^{n} p(X_i|\theta) \, d\theta$$

and

$$G_n = -\int q(x) \log p(x|X^n) \, dx.$$

Then $\mathbb{E}[F_n|q]$ satisfies

$$\mathbb{E}[F_n|q] = \text{KL}(q(x^n)||p(x^n)) + nS(q),$$
Then it follows that

\[
\text{KL}(q(x^n)||p(x^n)) = \int q(x^n) \log \frac{q(x^n)}{p(x^n)} \, dx^n,
\]

and \(q(x^n) = \prod_{i=1}^n q(x_i)\). Therefore, \(E[F_n|q]\) is minimized at \(q(x^n) = p(x^n)\). Also \(E[G_n|q]\) satisfies

\[
E[G_n|q] = \text{KL}(q(x)||p(x|x^n)) + S(q), \tag{2.13}
\]

where \(\text{KL}(q(x)||p(x|x^n))\) is the conditional Kullback–Leibler divergence

\[
\text{KL}(q(x)||p(x|x^n)) = \int q(x) q(x^n) \log \frac{q(x)}{p(x|x^n)} \, dx \, dx^n.
\]

Therefore, \(E[G_n|q]\) is minimized at \(q(x) = p(x|x^n)\). These two properties show that both the average free energy and the average generalization loss can be employed as measures of appropriateness of the candidate pair given by equations (2.1) and (2.2) with respect to \(q(x)\). In general, for an arbitrary positive integer \(n\)

\[
E[G_n|q] = E[F_{n+1}|q] - E[F_n|q] \tag{2.14}
\]

holds, however, minimization of the free energy gives the different result from that of the generalization loss.

Also we can define two functionals of a candidate pair \((p(x|\theta), \pi(\theta))\),

\[
\mathcal{F}(p, \pi) = \int E[F_n|q] \, dQ(q) \tag{2.15}
\]

and

\[
\mathcal{G}(p, \pi) = \int E[G_n|q] \, dQ(q). \tag{2.16}
\]

Then it follows that

\[
\mathcal{F}(p, \pi) = -\int \bar{q}(x^n) \log \bar{q}(x^n) \, dx^n + \int \log \bar{q}(x^n) \log \frac{\bar{q}(x^n)}{p(x^n)} \, dx \, dx^n \tag{2.17}
\]

and

\[
\mathcal{G}(p, \pi) = -\int \bar{q}(x^n) \bar{q}(x|x^n) \int \log \bar{q}(x|x^n) \, dx \, dx^n + \int \bar{q}(x^n) \bar{q}(x|x^n) \log \frac{\bar{q}(x|x^n)}{p(x|x^n)} \, dx \, dx^n, \tag{2.18}
\]

where

\[
\bar{q}(x^n) = \int q(x^n) \, dQ(q) \tag{2.20}
\]

and

\[
\bar{q}(x|x^n) = \frac{\int q(x)q(x^n) \, dQ(q)}{\int q(x^n) \, dQ(q)}. \tag{2.21}
\]

Therefore, both \(\mathcal{F}(p, \pi)\) and \(\mathcal{G}(p, \pi)\) are minimized if \(q(x) = p(x|\theta)\) and \(Q(q) = \pi(\theta)\). If a candidate pair \((p(x|\theta), \pi(\theta))\) happens to be completely equal to the unknown \((q(x), Q(q))\), then it is optimal from both viewpoints of \(\mathcal{F}(p, \pi)\) and \(\mathcal{G}(p, \pi)\). However, if a candidate one is not completely equal to the unknown one, two evaluations \(\mathcal{F}(p, \pi)\) and \(\mathcal{G}(p, \pi)\) are not equivalent to each other.

For given probability distributions \(p(x|\theta)\) and \(q(x)\), the average and empirical log loss functions, which are equal to the average and empirical average of the minus log-likelihood functions,
respectively, are defined by

\[ L(\theta) = -\int q(x) \log p(x|\theta) \, dx \]  \hspace{1cm} (2.22)

and

\[ L_n(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \log p(X_i|\theta). \]  \hspace{1cm} (2.23)

Let \( \Theta_0 \) be the set of all parameters that minimize \( L(\theta) \), and \( \theta_0 \) be an element of \( \Theta_0 \). In general, \( \Theta_0 \) may consist of multiple elements and the Hessian matrix of \( L \) need not be positive definite. If \( \Theta_0 \) consists of a single element and the Hessian matrix at \( \theta_0 \) is positive definite, then \( q(x) \) is said to be regular for \( p(x|\theta) \), if otherwise singular. For example, in overparametrized models such as normal mixtures, neural networks and many learning machines, \( \Theta_0 \) is an analytic or algebraic set with singularities [17]. In singular cases, the posterior distribution cannot be approximated by any normal distribution even if \( n \) is sufficiently large. In this paper, we assume that \( \Theta_0 \) consists of multiple elements in general and that \( p(x|\theta_0) \) does not depend on the choice of \( \theta_0 \in \Theta_0 \). Two variables \( L_0 \) and \( L_{0,n} \) are defined by \( L_0 = L(\theta_0) \) and \( L_{0,n} = L_n(\theta_0) \), which are called the average and empirical log losses of a parameter \( \theta_0 \), respectively. For the case when \( p(x|\theta_0) \) depends on \( \theta_0 \), see [18,19]. If there exists \( \theta_0 \) such that \( q(x) = p(x|\theta_0) \), then \( q(x) \) is said to be realizable by \( p(x|\theta) \). If \( q(x) \) is realizable by \( p(x|\theta) \), then \( S(q) = L_0 \) and \( S_n(q) = L_{0,n} \). The following concept RLCT is defined in both cases when \( q(x) \) is unrealizable by and singular for a statistical model \( p(x|\theta) \).

**Definition of RLCT.** For a given triple, \((p(x|\theta), \pi(\theta), q(x))\), a zeta function of Bayesian statistics is defined by

\[ \zeta(z) = \int (L(\theta) - L_0)^2 \pi(\theta) \, d\theta, \]  \hspace{1cm} (2.24)

where \( z \in \mathbb{C} \) is one complex variable. If \( L(\theta) \) is a piecewise analytic function of \( \theta \), then \( \zeta(z) \) is a holomorphic function in the region \( \Re(z) > 0 \), which can be analytically continued to the unique meromorphic function on the entire complex plane [17,20,21]. It is proved that all poles of \( \zeta(z) \) are real and negative numbers. Let \( -\lambda (\lambda > 0) \) be the largest pole of \( \zeta(z) \) and \( m \) be its order. The constants \( \lambda \) and \( m \) are called the RLCT and multiplicity.

The concept RLCT is a well-known birational invariant in algebraic geometry, which plays an important role also in Bayesian statistics. If \( q(x) \) is regular for a statistical model, then \( \lambda = d/2 \) and \( m = 1 \), where \( d \) is the dimension of the parameter space. For examples of RLCTs of singular statistical models, see §6b.

**Geometric Understanding of RLCT.** It has a clear geometric meaning. In fact, we can prove [17] that

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

where \( \Prob(\varepsilon) \) is the probability of the set of almost optimal parameters measured by the prior distribution,

\[ \Prob(\varepsilon) = \int_{L(\theta) < L_0 + \varepsilon} d\pi(\theta). \]

Since this probability is equal to an invariant of singularities, the statistical estimation performance of the Bayesian inference is determined by a kind of volume dimension of an analytic or an algebraic set. Note that, the smaller the probability is, the larger RLCT is, since \( \log \varepsilon \to -\infty \). It was proved that, if \( 0 < \pi(\theta) < \infty \) on \( \Theta_0 \), then \( \lambda \) does not depend on the choice of \( \pi(\theta) \) and singularities in \( \Theta_0 \) make the probability larger than the regular points, hence RLCT is smaller. If \( \pi(\theta_0) = 0 \) or \( \infty \) at \( \theta_0 \in \Theta_0 \) by controlling a hyperparameter, then \( \lambda \) depends on the hyperparameter. It may be an important fact that Jeffreys’ prior is equal to zero at singularities because the Fisher information matrix contains zero eigenvalue.
3. Cross validation and information criterion

(a) Adjusted cross validation

In this section, we study statistical inference about the generalization loss $G_n$. Let us define a training loss $T_n$, an LOO cross validation loss $C_n$ and a WAIC $W_n$, respectively, by

\[ T_n = -\frac{1}{n} \sum_{i=1}^{n} \log p(X_i|X^n), \tag{3.1} \]

\[ C_n = -\frac{1}{n} \sum_{i=1}^{n} \log p(X_i|X^n \setminus X_i), \tag{3.2} \]

\[ W_n = T_n + \frac{1}{n} \sum_{i=1}^{n} \mathbb{V}_\theta[\log p(X_i|\theta)], \tag{3.3} \]

where $p(x|X^n)$ is the posterior predictive distribution defined by equation (2.4), $X^n \setminus X_i$ is the sample leaving $X_i$ out from $X^n$ and $\mathbb{V}_\theta[\ ]$ is the variance about $\theta$ in the posterior distribution equation (2.3), which is, for an arbitrary function $f(\theta)$,

\[ \mathbb{V}_\theta[f(\theta)] = \int f(\theta)^2 p(\theta|X^n) \, d\theta - \left( \int f(\theta) p(\theta|X^n) \, d\theta \right)^2. \]

Note that $T_n$, $C_n$ and $W_n$ are defined without using any information about $q(x)$.

Then even if $q(x)$ is not realizable by $p(x|\theta)$ and even if $q(x)$ is singular for $p(x|\theta)$, the following properties are proved [14,22]. Based on algebraic geometrical method, there exist random variables $R_1$ and $R_2$ such that

\[ G_n = L_0 + \left( \lambda + R_1 - R_2 \right) \frac{1}{n} + o_p \left( \frac{1}{n} \right), \tag{3.4} \]

\[ T_n = L_{0,n} + \left( \lambda - R_1 - R_2 \right) \frac{1}{n} + o_p \left( \frac{1}{n} \right), \tag{3.5} \]

\[ C_n = L_{0,n} + \left( \lambda - R_1 + R_2 \right) \frac{1}{n} + o_p \left( \frac{1}{n} \right), \tag{3.6} \]

\[ W_n = L_{0,n} + \left( \lambda - R_1 + R_2 \right) \frac{1}{n} + o_p \left( \frac{1}{n} \right), \tag{3.7} \]

where $R_1$ and $R_2$ satisfy $\mathbb{E}[R_1] = \mathbb{E}[R_2] + o(1)$ and

\[ R_2 = \frac{1}{2} \sum_{i=1}^{n} \mathbb{V}_\theta[\log p(X_i|\theta)] + o_p(1). \]

The concrete forms of $R_1$ and $R_2$ are given in [22], in theorem 6 for regular cases and theorem 14 for singular cases. The convergences in distribution of $R_1$ and $R_2$ are proved using the empirical process theory for renormalized log-likelihood functions. These equations show that the generalization loss can be estimated by LOO cross validation and WAIC. Both $C_n$ and $W_n$ are asymptotically unbiased estimators of $G_n$, whereas neither AIC nor DIC [23] is. Note that if $X^n$ is a set of independent random variables, then LOO and WAIC are asymptotically equivalent, if otherwise not. For the differences between LOO and WAIC, see §6.

These equations (3.4)–(3.7) show a good behaviour of the LOO cross validation and the WAIC, however, $G_n - L_0$ and $C_n - L_{0,n}$ have an inverse correlation to each other [14,22],

\[ (G_n - L_0) + (C_n - L_{0,n}) = \frac{2\lambda}{n} + o_p \left( \frac{1}{n} \right). \]

Also $G_n - L_0$ and $W_n - L_{0,n}$ satisfy the same equation, which is the disadvantage of both LOO and WAIC. It should be emphasized that many statisticians may not be aware of this weak
The hold-out cross validation or the out-of-sample cross validation is defined by

\[ C_n = -\frac{1}{n} \sum_{i=1}^{n_1} \log p(X_i | X_{n_1} \setminus X_i). \]

Then it follows that

\[ \mathbb{E}[C_n] = L_0 + \frac{\lambda}{n_1} + o \left( \frac{1}{n_1} \right). \]

The hold-out cross validation or the out-of-sample cross validation is defined by

\[ H_{n_2} = -\frac{1}{n_2} \sum_{i=n_1+1}^{n} \log p(X_i | X_{n_1}^{n_2}), \]  

(3.8)

which estimates the generalization loss of the posterior predictive distribution made by \( X_{n_1} \) that is measured by using \( X_{n_2} \). This is an asymptotic unbiased estimator of \( G_{n_1} \),

\[ \mathbb{E}[H_{n_2}] = L_0 + \frac{\lambda}{n_1} + o_p \left( \frac{1}{n_1} \right). \]

An adjusted cross validation (ACV) is proposed by a weighted sum of the LOO and hold-out cross validations,

\[ A_n = \frac{n_1}{n} C_n + \frac{n_2}{n} H_{n_2}. \]  

(3.9)

By the definition, \( A_n \) is an asymptotic unbiased estimator of the generalization loss \( G_{n_1} \),

\[ \mathbb{E}[A_n] = L_0 + \frac{\lambda}{n_1} + o \left( \frac{1}{n_1} \right). \]

It follows that

\[ \frac{n_1}{n} \mathbb{E}[A_n - L_{0,n}] = \mathbb{E}[G_n - L_0] + o \left( \frac{1}{n} \right), \]

which shows that \((n_1/n)(A_n - L_{0,n})\) is an asymptotic unbiased estimator of \( G_n - L_0 \). Moreover, \( A_n - L_{0,n} \) does not have an inverse correlation to \( G_{n_1} - L_0 \), hence it provides the better estimator than \( C_n - L_{0,n} \) and \( W_n - L_{0,n} \), if the average of the 1/n order term of \( G_{n_1} \) is equal to that of \( G_n \). For theoretical foundation in regular cases, see §3c. Note that, in the evaluation of prior distributions on the condition that a statistical model is fixed, then the 1/n order terms are common and the compared terms have higher order than 1/n, resulting that the adjusted cross validation may not be a better measure than LOO and WAIC. The higher-order probabilistic behaviours of the generalization loss, LOO and WAIC, are shown in §5.

The rescaled hold-out or out-of-sample cross validation error

\[ \frac{n_1}{n} (H_{n_2} - L_{0,n_2}) = -\frac{1}{n} \sum_{i=n_1+1}^{n} (\log p(X_i | X_{n_1}^{n_2}) - \log q(X_i)) \]

is also an unbiased estimator of \( G_n - L \), which has the larger variance than \((n_1/n)(A_n - L_n)\). Note that, if a probability distribution \( q(x) \) is realizable by \( p(x|\theta) \), then neither \( L_0 = S(q) \) nor \( L_{0,n} = S_n(q) \) depends on \( p(x|\theta) \) and \( \pi(\theta) \).
(b) Numerical experiment

In this subsection, we show a numerical experiment.

**Example 3.1.** In order to illustrate the differences of the several estimators of the generalization loss, a matrix factorization problem is studied. Let \( X, A \) and \( B \) be \( M \times N \), \( M \times H \) and \( H \times N \) matrices, respectively. A statistical model and a prior distribution of a matrix factorization are defined by

\[
p(X|A, B) \propto \exp\left(-\frac{1}{2} ||X - AB||^2\right)
\]

(3.10)

and

\[
\pi(A, B) \propto \exp\left(-\frac{1}{2 \rho^2} ||A||^2 - \frac{1}{2 \mu^2} ||B||^2\right),
\]

(3.11)

where \( || \cdot || \) is the Frobenius norm and \( \rho, \mu > 0 \) are hyperparameters. This model is sometimes employed for the purpose that a random matrix \( X \) is estimated by a product of low rank matrices \( A \) and \( B \). Since the map \((A, B) \mapsto p(x|A, B)\) is not one-to-one, this model is not regular but singular. The posterior distribution cannot be estimated by any normal distribution. The real log canonical threshold \( \lambda \) of this model is the same as that of the reduced rank regression which was clarified in [24]. In the experiment, we studied a case when \( M = N = 8 \), \( \rho = \mu = 0.12 \). A sample \( X^n (n = 200) \) was taken from \( q(X) = p(X|A_0, B_0) \), where \( A_0B_0 = \text{diag}(1, 1, 0, 0, 0, 0, 0, 0) \) is a diagonal matrix. Hence the rank of \( A_0B_0 \) is \( H_0 = 2 \). We conducted two experiments \( H = 2 \) and \( H = 6 \). If \( H = 2 \), the model is appropriate for \( H_0 \), but if \( H = 6 \), the model is over-parametrized. The values RLCIs for \( H = 2 \) and \( H = 6 \) are \( \lambda = 14 \) and \( \lambda = 24 \), respectively, whereas half of the dimensions of the parameter spaces \( d/2 = (MH + HN - N^2)/2 \) are 14 and 30, respectively. Two hundred independent trials were conducted. In experimental comparison, the average and empirical entropies of \( q(X) \) are reduced from the estimators. Let the generalization error be \( \text{GE. E.} = G_n - S \), the cross validation error, the WAIC error, the ACV error, the hold-out cross validation error, the AIC error and the DIC [23] error are, respectively, defined by reducing the empirical entropy.

- **LOO. E.** = \( C_n - S_n(q) \),
- **WAIC. E.** = \( W_n - S_n(q) \),
- **AC. E.** = \( \left( \frac{n_1}{n} \right) (A_n - S_n(q)) \),
- **HO. E.** = \( \left( \frac{n_2}{n} \right) (H_n - S_n(q)) \),
- **AIC. E.** = \( \text{AIC} - S_n(q) \),
- **DIC. E.** = \( \text{DIC} - S_n(q) \).

(3.12)  (3.13)  (3.14)  (3.15)  (3.16)  (3.17)

Note that \( A_n - S_n(q) \) and \( H_n - S_n(q) \) are estimators of \( E[G_{n_1}] - S(q) \), they are used as estimators of \( E[G_n] - S(q) \) by rescaling. In calculation of the adjusted and hold-out cross validations, we used \( n_1 = n_2 = 100 \). In table 1, in the case \( H = 2 \), the six values from \( \text{GE. E.} \) to \( \text{AIC. E.} \) have asymptotically the same expectation values \( \lambda/n = 0.07 \). In the case \( H = 6 \), the five values from \( \text{GE. E.} \) to \( \text{HO. E.} \) have asymptotically the same expectation values \( \lambda/n = 0.12 \), whereas neither \( \text{AIC. E.} \) nor \( \text{DIC. E.} \) does. These results are caused by the fact that matrix factorization is a singular statistical model and the posterior distribution cannot be approximated by any normal distribution. In the table, \( \text{MEAN} \) and \( \text{STD} \) show averages and standard deviations of these random variables, and RSE shows the root square errors of the generalization error and estimated errors, \( E[(\text{GE. E.} - \text{LOO. E.})^2]^{1/2}, E[(\text{GE. E.} - \text{WAIC. E.})^2]^{1/2}, \) and so on. These experimental results show the ACV is a better estimator of the generalization loss than the other estimators, because it has the smallest standard deviation and root square error in both cases \( H = 2 \) and \( H = 6 \).
Table 1. Comparison of Estimators of Generalization Error. GE.E.: Generalization error, LOO.E.: Leave-one-out error, WAIC.E.: Widely applicable information criterion error, AIC.E.: Adjusted cross validation error, HO.E.: Hold-out cross validation error, DIC.E.: Akaike information criterion error, E.: Deviance information criterion error.

|               | $H_0 = H = 2$                                      | $H_0 = 2, H = 6$                                      |
|---------------|---------------------------------------------------|---------------------------------------------------|
|               | mean  | s.d.   | RSE   | mean  | s.d.   | RSE   |
| GE. E.        | 0.071 | 0.019  | 0.117 | 0.025 |
| LOO. E.       | 0.069 | 0.018  | 0.037 | 0.024 | 0.049 |
| WAIC. E.      | 0.069 | 0.018  | 0.037 | 0.024 | 0.049 |
| AIC. E.       | 0.071 | 0.014  | 0.031 | 0.017 | 0.039 |
| HO. E.        | 0.074 | 0.032  | 0.043 | 0.040 | 0.053 |
| AIC. E.       | 0.068 | 0.018  | 0.037 | 0.015 | 0.062 |
| DIC. E.       | −5.492 | 11.432 | 12.688 | −1.262 | 0.505 | 1.469 |

(c) Variances of cross validations in regular case

In this subsection, we theoretically compare the adjusted cross validation $A_n$ and the LOO cross validation $C_n$ when $q(x)$ is regular for $p(x|\theta)$. Since $(n_1/n)(A_n - L_0)$ and $C_n - L_0$, are asymptotic unbiased estimators of the generalization error $G_n - L_0$, we show that the variance of $(n_1/n)(A_n - L_0)$ is smaller than that of $C_n - L_0$, on the assumption both $n_1/n$ and $n_2/n$ converge to constants. For the case when $q(x)$ is not regular for $p(x|\theta)$, theoretical comparison is still an open problem.

As we assumed the regularity condition, $\theta_0$ is unique and the Hessian matrix $J = \nabla^2 L(\theta_0)$ is positive definite. We define a matrix $I$ by

$$I = \int \nabla \log p(x|\theta_0) (\nabla \log p(x|\theta_0))^T q(x) \, dx,$$

where $T$ shows the transpose of the vector. Then based on just the same method as chapter 4, theorem 6, in [22], the LOO and hold-out cross validations, $C_{n_1}$ and $H_{n_2}$, are asymptotically derived as

$$C_{n_1} = L_{0,n_1} + \frac{1}{2n_1} \left( -||\xi_{n_1}||^2 + d + \text{tr}(JJ^{-1}) \right) + O_P(n_1^{-3/2})$$

and

$$H_{n_2} = L_{0,n_2} + \frac{1}{2n_2} \left( -2\sqrt{\frac{n_1}{n_2}} \xi_{n_1} \cdot \eta_{n_2} + ||\xi_{n_1}||^2 + d - \text{tr}(JJ^{-1}) \right) + O_P(n_1^{-3/2}),$$

where $\xi_{n_1}$ and $\eta_{n_2}$ are $\mathbb{R}^d$-valued independent random variables,

$$\xi_{n_1} \equiv -J^{-1/2} \frac{1}{\sqrt{n_1}} \sum_{i=1}^{n_1} \nabla \log p(X_i|\theta_0)$$

and

$$\eta_{n_2} \equiv -J^{-1/2} \frac{1}{\sqrt{n_2}} \sum_{i=n_1+1}^{n} \nabla \log p(X_i|\theta_0),$$

which converge in distribution to the same normal distribution with average 0 and covariance matrix $J^{-1/2}J^{-1/2}$. Consequently

$$\mathbb{E}[||\xi_{n_1}||^2] \rightarrow \text{tr}(JJ^{-1}),$$

$$\mathbb{E}[||\xi_{n_1}||^4] - \mathbb{E}[||\xi_{n_1}||^2]^2 \rightarrow 2\text{tr}((JJ^{-1})^2),$$

$$\mathbb{E}[(\xi_{n_1} \cdot \eta_{n_2})^2] \rightarrow \text{tr}((JJ^{-1})^2).$$
By the definition of $C_n$ in equation (3.2) and $A_n$ in equation (3.9), the asymptotic variances of $C_n - L_{0,n}$ and $(n_1/n)(A_n - L_{0,n})$ are given by equations (3.23)–(3.25), resulting in:

$$V[C_n - L_{0,n}] = \frac{1}{2n^2} \text{tr}((IJ^{-1})^2) + o(n^{-2})$$  \hspace{1cm} (3.26)

and

$$V\left[\left(\frac{n_1}{n}\right)(A_n - L_{0,n})\right] = \frac{1}{2n^4}(n_1^2 + n_2^2)\text{tr}((IJ^{-1})^2) + o(n^{-2}).$$  \hspace{1cm} (3.27)

Hence the asymptotic variance of $(n_1/n)(A_n - L_{0,n})$ is made smallest when $n_1 = n_2 = n/2$ and the variance in the smallest case is half of that of $C_n$.

**Remark.** As a consequence of this theoretical result, if $q(x)$ is regular for $p(x|\theta)$, the same method can be extended. Let $n$ be quite large and let $A_{n/2}$ and $A'_{n/2}$ be adjusted cross validations calculated from $(X_1, X_2, \ldots, X_{n/2})$ and $(X_{n/2+1}, X_{n/2+2}, \ldots, X_n)$, respectively. Then the following three random variables have asymptotically the same expectation value as $E[G_n] - L_0 \approx \text{tr}(IJ^{-1})/(2n)$,

$$C_n - L_{0,n}, \hspace{1cm} \left(\frac{1}{2}\right)(A_n - L_{0,n}) \hspace{1cm} (3.28)$$

and

$$\left(\frac{1}{8}\right)(A_{n/2} + A'_{n/2} - L_{0,n}), \hspace{1cm} (3.30)$$

whereas the ratio of their variances is $(1 : 1/2 : 1/4)$. The same method can be generalized for arbitrary partition of a sample, resulting that the variance can be made arbitrary smaller. However, if a partition makes each sample size of each ACV too small, the asymptotic evaluation $E[G_m] - L_0 \approx \text{tr}(IJ^{-1})/(2m)$ for large $m$ may not be satisfied. This is a problem of bias and variance in the estimation of the generalization error. It is the future study to clarify the optimal number of partitions for a large $n$.

### 4. Marginal likelihood and free energy

In this section, several approximations of the free energy which is the minus log marginal likelihood equation (2.10) are compared. Even if $q(x)$ is not realizable by $p(x|\theta)$ or even if the posterior distribution cannot be approximated by any normal distribution, it is derived [17] that

$$F_n = nL_{0,n} + \lambda \log n - (m - 1) \log \log n + O_p(1),$$

where $\lambda$ and $m$ are RLCT and its multiplicity, respectively.

By equation (2.14), the constant term of the free energy does not affect the generalization loss. In fact, the asymptotic balances of biases and variances are given by

$$E[F_n|q] = nL_0 + \lambda \log n$$  \hspace{1cm} (4.1)

and

$$n \times E[G_n|q] = nL_0 + \lambda,$$  \hspace{1cm} (4.2)

hence the variance term $\lambda \log n$ of the free energy is larger than $\lambda$ of the generalization loss. In other words, optimizations for the free energy and the generalization loss are incompatible with each other. According to the increase of sample size $n$, the different balance of the bias and variance affect the generalization performance [25].

In general, it needs heavy computational cost to calculate the numerical value of the free energy, hence several methods have been developed. If a statistical model is regular, then BIC
Table 2. Estimators of Free Energy. AFE/n: Asymptotic free energy divided by $n$, BIC/n: Bayesian information criterion divided by $n$, WBIC/n: Widely applicable information criterion divided by $n$.

|                  | $H_0 = H = 2$ |                  | $H_0 = 2, H = 6$ |
|------------------|---------------|------------------|------------------|
|                  | mean | s.d. | mean | s.d. |
| AFE/n—$S_n$      | 0.30 | 0.02 | 0.48 | 0.03 |
| BIC/n—$S_n$      | 0.30 | 0.02 | 0.64 | 0.03 |
| WBIC/n—$S_n$     | 0.31 | 0.02 | 0.49 | 0.02 |

[16] is defined by

$$BIC = nL_n(\hat{\theta}) + \frac{d}{2} \log n,$$

where $\hat{\theta}$ is the maximum-likelihood estimator. The asymptotically main term of the free energy (AFE) is given by

$$AFE = nL_n(\hat{\theta}) + \lambda \log n.$$

In general, RLCT depends on $(q(x), p(x|\theta), \pi(\theta))$, this equation cannot be used directly if $q(x)$ is unknown. The generalized version of BIC onto singular cases was proposed by using the estimated RLCT $\hat{\lambda}$ [26],

$$sBIC = nL_n(\hat{\theta}) + \hat{\lambda} \log n.$$

This method $sBIC$ needs theoretical results about RLCTs but does not need Markov chain Monte Carlo (MCMC) approximation of the posterior distribution. By using the MCMC sample of the parameter, another method was developed. A posterior distribution of the inverse temperature $\beta > 0$ is defined by

$$\mathbb{E}_\theta(\beta)[f(\theta)] = \frac{\int f(\theta)\pi(\theta) \prod_{i=1}^n p(X_i|\theta)^\beta \, d\theta}{\int \pi(\theta) \prod_{i=1}^n p(X_i|\theta)^\beta \, d\theta}.$$

Then WBIC is defined by $\beta = 1/\log n$ [27,28]

$$WBIC = \mathbb{E}_\theta^{(1/\log n)}[nL_n(\theta)],$$

which satisfies

$$WBIC = nL_0,n + \lambda \log n + o_p(\log n).$$

Also it is proved that, if the posterior distribution can be approximated by a normal distribution, then

$$WBIC = BIC + o_p(1).$$

Note that BIC, asymptotic free energy (AFE) and WBIC approximate the log $n$ order term of the free energy, hence their values have constant order differences from the free energy. The prior distribution does not affect their values directly if it does not change RLCT, whereas it does the constant order term.

**Example 4.1.** Let us compare BIC, WBIC and asymptotic form of the free energy. The asymptotic form is equal to $sBIC$ if $\hat{\lambda} = \lambda$. A matrix factorization problem same as example 3.1 was studied. For $M, N, H, H_0, n$ and $A_0B_0$, the same condition as example 3.1 was conducted. We compared $AFE/n - S_n(q)$, $BIC/n - S_n(q)$ and $WBIC/n - S_n(q)$. Table 2 shows their averages and standard deviations. When $H = H_0$, then three values coincided with each other, whereas in a singular case $H > H_0$, then they were different. The experimental result shows that WBIC approximated the asymptotic from better than BIC in overparametrized cases.
5. Evaluation of prior distributions

In this section, we study the relation between prior distributions and generalization losses, on the assumption that a statistical model \( p(x|\theta) \) is regular and fixed, that is to say, for an arbitrary \( \theta \), the Hessian matrix of \( L(\theta) \) is positive definite.

We consider a condition that a candidate prior distribution \( \pi(\theta) \geq 0 \) may be improper, that is to say, in general,

\[
\int \pi(\theta) \, d\theta = \infty.
\]

Even if it is improper, the posterior and posterior predictive distributions can be defined by equations (2.3) and (2.4) if both are finite. The generalization loss \( C_n(\pi) \), the LOO cross validation \( C_n(\pi) \), the WAIC \( W_n(\pi) \), the hold-out cross validation \( H_n(\pi) \) and the adjusted cross validation \( \Lambda_n(\pi) \) can also be defined by the same equations (2.11), (3.2), (3.3), (3.8) and (3.9), respectively. However, if a prior distribution is improper, the marginal likelihood cannot be a measure of the appropriateness of the prior distribution, because it may be made infinite by choosing an improper prior distribution.

In this section, we fix a statistical model \( p(x|\theta) \) and study the effect of a candidate prior distribution \( \pi(\theta) \). The function \( q(x) \) is assumed to be unrealizable by a statistical model in general. Let \( \pi_0(\theta) > 0 \) be an arbitrary fixed non-negative function on \( \mathbb{R}^d \). For example, one can choose \( \pi_0(\theta) \equiv 1 \) for an arbitrary \( \theta \). For a given \((\pi(\theta), \pi_0(\theta))\), a function \( \phi(\theta) \) is defined by

\[
\phi(\theta) = \frac{\pi(\theta)}{\pi_0(\theta)}.
\]

On the foregoing assumptions, it is proved in \([22,29]\) that there exists a function \( M(\phi, \theta) \) such that

\[
\mathbb{E}[G_n(\pi)|q] = \mathbb{E}[G_n(\pi_0)|q] + \frac{M(\phi, \theta_0)}{n^2} + o\left(\frac{1}{n^2}\right),
\]

(5.1)

\[
\mathbb{E}[C_n(\pi)|q] = \mathbb{E}[C_n(\pi_0)|q] + \frac{d/2 + M(\phi, \theta_0)}{n^2} + o\left(\frac{1}{n^2}\right),
\]

(5.2)

\[
\mathbb{E}[W_n(\pi)|q] = \mathbb{E}[G_n(\pi_0)|q] + \frac{d/2 + M(\phi, \theta_0)}{n^2} + o\left(\frac{1}{n^2}\right),
\]

(5.3)

where \( \theta_0 \) is the parameter that minimizes \( L(\theta) \) in equation (2.22). That is to say, the expectation values of the generalization loss, the LOO cross validation and WAIC are equivalent in the higher order. Also it was proved in \([22,29]\) that there exists a function \( M(\phi, \theta) \) of \( \phi(\theta) \) and \( \theta \) which satisfies

\[
C_n(\pi) = C_n(\pi_0) + \frac{M(\phi, \hat{\theta})}{n^2} + o_p\left(\frac{1}{n^2}\right),
\]

(5.4)

and

\[
W_n(\pi) = W_n(\pi_0) + \frac{M(\phi, \hat{\theta})}{n^2} + o_p\left(\frac{1}{n^2}\right),
\]

(5.5)

where \( \hat{\theta} \) is the parameter that maximizes \( \pi_0(\theta) \prod_{i=1}^n p(X_i|\theta) \), in other words, \( \hat{\theta} \) is the maximum a posteriori estimator for a fixed prior function \( \pi_0(\theta) \). Hence LOO and WAIC are also equivalent in the higher order as random variables. The concrete forms of the functionals \( M(\phi, \theta) \) and \( M(\phi, \theta) \) are defined by using higher order differential geometric forms of the log density function \( \log p(x|\theta) \) \([22,29]\). They satisfy

\[
M(\phi, \hat{\theta}) = M(\phi, \theta_0) + o_p\left(\frac{1}{n^{1/2}}\right),
\]

(5.6)

\[
M(\phi, E_\theta[\theta]) = M(\phi, \hat{\theta}) + o_p\left(\frac{1}{n}\right),
\]

(5.7)

\[
\mathbb{E}[M(\phi, \hat{\theta})] = M(\phi, \theta_0) + O\left(\frac{1}{n}\right).
\]

(5.8)
It should be emphasized that the generalization loss as a random variable has the different behaviour from its own average [29]

$$G_n(\pi) = G_n(\pi_0) + O_p\left(\frac{1}{n^{3/2}}\right).$$ (5.9)

The parameter that minimizes the average generalization loss does not minimize the random generalization loss. Also minimization of WAIC or LOO by choosing $\pi(\theta)$ makes the average generalization loss $E[G_n(\pi)]$ minimized asymptotically, however, it does not minimize the generalization loss $G_n(\pi)$ as a random variable.

The free energy or the marginal likelihood has the different behaviour than the cross validation and information criterion. Let $F_n(\pi)$ be the free energy of a proper prior distribution. Assume that $\pi(\theta)$ and $\pi_0(\theta)$ satisfy $\int \pi(\theta) \, d\theta = \int \pi_0(\theta) \, d\theta = 1.$ Then it follows that [30]

$$F_n(\pi) = F_n(\pi_0) - \log \frac{\pi(\theta_0)}{\pi_0(\theta_0)} + o_p(1)$$ (5.10)

$$= F_n(\pi_0) - \log \frac{\pi(\theta_{\text{mle}})}{\pi_0(\theta_{\text{mle}})} + o_p(1),$$ (5.11)

where $\theta_{\text{mle}}$ is the maximum-likelihood estimator. Hence the minimization of $F_n(\pi)$ is asymptotically equivalent to maximization of $\pi(\theta_{\text{mle}})$ at the maximum-likelihood estimator.

If a set of candidate prior distributions is given by $[\pi(\theta|a); a]$, where $a$ is a hyperparameter, the optimal hyperparameter that is determined by minimization of $F_n(\pi(\theta|a))$ does not converge to the parameter that minimizes the average generalization loss in general even if the sample size tends to infinity. For example, a statistical model $p(x|m, s)$ and a prior distribution $\pi(m, s|a)$, where $a > 0$ is a hyperparameter, are given by

$$p(x|m, s) = \sqrt{\frac{s}{2\pi}} \exp\left(-\frac{s}{2}(x - m)^2\right)$$ (5.12)

and

$$\pi(m, s|a) = \frac{a}{2\sqrt{2\pi s}} \exp\left(-\frac{s}{2}(m^2 + a)\right),$$ (5.13)

and $q(x) = p(x|0, 1)$. Then by using the same method as section 2.1 in [22] and notations $A = \sum X_i^2$, $B = \sum X_i$, the free energy and the LOO cross validation are derived as, respectively, by

$$F_n(a) = -\log a + \frac{n + 1}{2} \log((A + a)(n + 1) - B^2) + C_1$$ (5.14)

$$C_n(a) = \frac{n + 1}{2} \log((A + a)(n + 1) - B^2)$$ (5.15)

$$- \frac{1}{2} \sum_{i=1}^{n} \log((A - X_i^2 + a)n - (B - X_i)^2) + C_2,$$ (5.16)

where either $C_1$ or $C_2$ does not depend on $a$. Hence the asymptotic analysis of the zero points of $F_n'(a)$ and $C_n'(a)$ shows that minimizers of $F_n(a)$ and $C_n(a)$ converge to the different values 2 and 4 as $n \to \infty$.

**Example 5.1.** A simple polynomial regression is studied. Let $x, y \in \mathbb{R}$ and $f(x) \in \mathbb{R}^K$, and $a \in \mathbb{R}^K$, where $K$ is a positive integer. Using a function

$$f(x) = (1, x, x^2, \ldots, x^{K-1})^T,$$

a pair of a statistical model and a prior distribution is defined by

$$p_k(y|x, a, s) = \left(\frac{s}{2\pi}\right)^{1/2} \exp\left(-\frac{s}{2}(y - a \cdot f(x))^2\right)$$ (5.17)

and

$$\pi(a, s|b, c, d) \propto s^{b-1} \exp\left(-cs - \frac{ds}{2}||a||^2\right).$$ (5.18)
In general, a sample $x^n$ is given from the real world, however, $x^n$ may or may not be a realization of some random variable in a real world. The terminology ‘uncertainty’ in this paper is used for the case when a person does not know whether $x^n$ is a realization of some random variable or not.

We study a case when a person who makes a special statistical model $p(x|\theta)$ and a special prior distribution $\pi(\theta)$ is aware they are fictional candidates, and wants to evaluate them from a more general viewpoint. It is a mathematical fact that the general pair $(q(x), Q(q))$ contains a special pair $(p(x|\theta), \pi(\theta))$ as a specific one, hence if a special pair exists, then the general pair also exists. The terminology ‘unknown information source’ in this paper is used for the case where a person does not know whether $x^n$ is a realization of some random variable or not.

We can understand that both pairs are prepared in a person’s mathematical analysis, which may be different from the real world. If the unknown general pair cannot be assumed to exist in the real world, then the evaluation by cross validation and information criteria shows the adequateness of a special pair in a person’s mathematical analysis and decision. If the unknown

### Table 3. Hyperparameter Optimization

| Optimized Hyper | Gen. Err. |
|-----------------|-----------|
| Mean | s.d. | Mean | s.d. |
| LOO.E. | 0.75 | 0.81 | 0.85 | 0.117 | 0.082 |
| WAIC.E. | 0.92 | 0.70 | 0.81 | 0.116 | 0.082 |
| AC.E. | 1.05 | 1.10 | 1.22 | 0.119 | 0.087 |
| HO.E. | 1.96 | 2.65 | 3.02 | 0.143 | 0.115 |
| Free.E. | 2.23 | 0.25 | 1.75 | 0.125 | 0.095 |

Note that the prior distribution is proper if and only if the hyperparameter $(b,c,d)$ satisfies $b > K/2$, $c > 0$, $d > 0$. Let $q(x)q(y|x)$ be a data-generating distribution where $q(x)$ is a standard normal distribution and $q(y|x) = p(y|x, a_0, s_0)$ with $a_0 = (1, -1/5, 1/30)$ and $s_0 = 25$. An experiment with $K = 3$ and $n = 20$ was conducted. The hyperparameter was set as $(b,c,d) = (b, 0.01, 0.01)$, where $b = -3, -2.5, -2, \ldots, 6.5$ are candidate hyperparameters. The optimal hyperparameter among them that minimizes $E[G(x)]$ is $b = 0.5$, which means the optimal one about $b$ makes the prior distribution improper. Two hundred independent trials were conducted. The optimal hyperparameters for LOO cross validation, WAIC, ACV, hold-out cross validation and the free energy were chosen and the generalization errors for the chosen hyperparameters were recorded. Table 3 shows averages, standard deviation and root square error of the optimized hyperparameters. Also the average and standard deviation of the corresponding generalization errors are shown.

The experimental results show that the LOO cross validation and the WAIC estimated the optimal hyperparameter better than the other methods and that the standard deviation of the chosen hyperparameters by WAIC was smaller than LOO. It would be helpful that minimization of the free energy is different from that of the generalization loss.

### 6. Discussion

In this section, we discuss three points in Bayesian statistics in this paper.

**(a) Uncertainty and information source in this paper**

In general, it seems that there are no mathematical definitions of ‘uncertainty’ and ‘information source’. In this subsection, the meaning of these words in this paper is explained.

In general, a sample $x^n$ is given from the real world, however, $x^n$ may or may not be a realization of some random variable in a real world. The terminology ‘uncertainty’ in this paper is used for the case when a person does not know whether $x^n$ is a realization of some random variable or not.

We study a case when a person who makes a special statistical model $p(x|\theta)$ and a special prior distribution $\pi(\theta)$ is aware they are fictional candidates, and wants to evaluate them from a more general viewpoint. It is a mathematical fact that the general pair $(q(x), Q(q))$ contains a special pair $(p(x|\theta), \pi(\theta))$ as a specific one, hence if a special pair exists, then the general pair also exists. The terminology ‘unknown information source’ in this paper is used for the case where a person does not know whether $x^n$ is a realization of some random variable or not.
general pair can be assumed to exist in the real world by some scientific background, then the evaluation by them has a scientifically objective meaning.

Note that the same mathematical theory holds even if the unknown general pair exists in the real world or not, and that no concrete information about the unknown information source is required in the use of the cross validation and information criteria. Hence, if a person cannot believe in a special pair, the evaluation by them is useful in both cases.

(b) Real log canonical threshold

In this subsection, we summarize researches about the RLCT.

If \( q(x) \) is regular for \( p(x|\theta) \), then \( \lambda = d/2, m = 1 \) and \( R_2 = \text{tr}(I^{-1})/2 \) in equation (2.11), where \( d \) is the dimension of the parameter space, \( I \) and \( J \) are defined in §3c. If \( q(x) \) is regular for and realizable by \( p(x|\theta) \), then \( 2R_1 \) is a random variable whose probability distribution converges to \( \chi^2 \) distribution with \( d \) degrees of freedom, and \( R_2 \) converges to \( d/2 \).

If a statistical model contains hierarchical structure or hidden variable, then it is in general singular. Such a statistical model is often prepared sufficiently large so that it can approximate an unknown information source, hence RLCTs in overparametrized cases are important in model evaluation.

The concrete values of RLCTs of singular statistical models have been clarified, for example, reduced rank regressions [24], neural networks [25,31], normal mixtures [32], Poisson mixtures [33], Latent Dirichlet allocations [34] and multinomial mixtures [35]. It is also clarified that, based on RLCT, the exchange probability of exchange MCMC methods can be optimally designed [36]. The mean field approximation of the posterior distribution is called the variational Bayesian inference. Both the generalization loss and the free energy of the variational Bayes approximation are clarified [37–39], which are different from the exact values even asymptotically. For the case when the data-generating process is not equal to singularities, the generalization performance was derived in [40].

(c) Comparison of cross validation and information criterion

In this subsection, we compare cross validation and information criterion from theoretical and computational points of view.

First, we compare cross validation and information criterion in not i.i.d. cases. If a sample is i.i.d. or exchangeable, then LOO cross validation and WAIC are asymptotically equivalent, if otherwise not. For example, in a regression problem where the conditional probability density \( \{q(Y_i|x_i)\} \) is estimated, \( \{x_i\} \) may be independent or not. If a probability distribution of \( \{Y_i\} \) for fixed \( \{x_i\} \) is given by

\[
\prod_{i=1}^{n} q(y_i|x_i),
\]

where \( \{x_i\} \) is not a random variable, then we define the generalization loss by

\[
C_n^{(1)} = \frac{1}{n} \sum_{i=1}^{n} \int dy q(y|x_i) \log p(y|x^n, Y^n).
\]

Otherwise if a probability distribution of \( \{(X_i, Y_i)\} \) is given by

\[
\prod_{i=1}^{n} q(x_i, y_i),
\]

then \( \{(X_i, Y_i)\} \) are independent. We define the generalization loss by

\[
C_n^{(2)} = \int dx \int dy q(x, y) \log p(y|X^n, Y^n).
\]
LOO and WAIC are asymptotically equivalent as the estimator of $G_{n}^{(2)}$ if $\{(X_i, Y_i)\}$ are independent. If $\{Y_i\}$ is independent but $\{X_i\}$ is fixed, WAIC can be used as an estimator of $G_{n}^{(1)}$, whereas LOO not. This difference becomes large if a leverage sample point is contained or the dimension of inputs $\{X_i\}$ is high [28]. Hence, for the cases when $\{Y_i\}$ are independent, then the ACV equation (3.9) should be defined by the replacement of $C_{n1}$ by $W_{ni}$. For general dependent cases such as time sequence analysis, the evaluation methods of the statistical models and prior distributions are not yet fully constructed, however, several measures which contain a specific statistical model, for example, the leave-future-out cross validation, were proposed [41].

Second, we study computational problems of cross validation and information criterion. In Bayesian inference, calculation of the LOO cross validation needs heavy computational costs because the posterior distributions for $X^n \setminus X_i$ are necessary for all $i = 1, 2, \ldots, n$. The importance sampling cross validation

$$\text{ISCV} = \frac{1}{n} \sum_{i=1}^{n} E_{\theta} \left[ \log \left( \frac{1}{p(X_i|\theta)} \right) \right] \quad (6.1)$$

can be used for numerical approximation. If a leverage sample point is contained in a sample, the posterior average or variance may be infinite [42,43], and a new estimation method has been proposed, which is useful in many practical problems [12,13,44,45].

### 7. Conclusion

We introduced a place of mathematical theory of Bayesian statistics when uncertainty is unknown. In almost all cases, a person who makes a pair of a statistical model and a prior distribution is aware that it is a fictional candidate. Therefore, a person needs statistical evaluation measures that can be employed even if an uncertainty is unrealizable or singular for a statistical model. Mathematical theory of a cross validation, an information criterion and a marginal likelihood will be one of the most important foundations for Bayesian statistics for unknown information source.

Data accessibility. The software used in this paper is available via: https://github.com/Sumio-Watanabe/Mathematical-Theory-of-Bayesian-Statistics-for-Unknown-Information-Source.

Author contributions. S.W.: conceptualization, data curation, formal analysis, funding acquisition, investigation, methodology, project administration, resources, software, supervision, validation, visualization, writing—original draft, writing—review and editing.

Conflict of interest declaration. I declare I have no competing interests.

Funding. This work was partially supported by JSPS Grant-in-Aid for Scientific Research (C) 21K12025.

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