Bayesian Cross Validation and WAIC for Predictive Prior Design in Regular Asymptotic Theory

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Abstract

Prior design is one of the most important problems in both statistics and machine learning. The cross validation (CV) and the widely applicable information criterion (WAIC) are predictive measures of the Bayesian estimation, however, it has been difficult to apply them to find the optimal prior because their mathematical properties in prior evaluation have been unknown and the region of the hyperparameters is too wide to be examined. In this paper, we derive a new formula by which the theoretical relation among CV, WAIC, and the generalization loss is clarified and the optimal hyperparameter can be directly found.

By the formula, three facts are clarified about predictive prior design. Firstly, CV and WAIC have the same second order asymptotic expansion, hence they are asymptotically equivalent to each other as the optimizer of the hyperparameter. Secondly, the hyperparameter which minimizes CV or WAIC makes the average generalization loss to be minimized asymptotically but does not the random generalization loss. And lastly, by using the mathematical relation between priors, the variances of the optimized hyperparameters by CV and WAIC are made smaller with small computational costs. Also we show that the optimized hyperparameter by DIC or the marginal likelihood does not minimize the average or random generalization loss in general.

Keywords. Hyperparameter, Cross validation, WAIC, DIC, marginal likelihood

1 Introduction

In statistics and machine learning, a method how to design a prior distribution is one of the most important problems. It is well known that Bayesian estimation or some regularization techniques are useful in practical statistical problems, however, its performance strongly depends on the prior, hence we need the theoretical foundation which enables us to evaluate the chosen prior.

Sometimes the parameter in the prior is called a hyperparameter, and the prior design problem results in the method how to choose the optimal hyperparameter. Historically, it was proposed that a hyperparameter is optimized by maximization of the marginal likelihood \([\text{Good, 1952}]. \text{Akaike, 1980}\). This method is one of the rational procedures because it can be understood as the maximum likelihood method for the marginal distribution,
however, the optimal prior for this criterion does not minimize the average generalization loss in general. In this paper, we study predictive prior design, in other words, a method how to choose a prior so as to minimize the average generalization loss.

The generalization loss can be estimated by the cross validation (CV) and information criteria. In Bayesian estimation, the leave-one-out cross validation can be approximated by using the important sampling cross validation [Gelfand et al., 1992; Vehtari and Lampinen, 2002], whose statistical property was studied in Bayesian statistics [Peruggia, 1997; Epifani et al., 2008; Vehtari and Ojanen, 2012]. The deviance information criterion (DIC) was proposed for the case when the true distribution is realizable by a statistical model and the posterior is a normal distribution [Spiegelhalter et al., 2002, 2014]. For general cases when the true distribution may be unrealizable or the posterior may not be a normal distribution, the widely applicable information criterion (WAIC) was proposed based on singular learning theory [Watanabe, 2001, 2009, 2010a] and it was proved that WAIC is asymptotically equivalent to the leave-one-out cross validation [Watanabe, 2010a]. Both CV and WAIC are studied by using the Hamiltonian Monte Carlo methods and its improved algorithm using No-U-Turn dynamics [Gelman et al., 2013, 2014; Vehtari and Ojanen, 2012].

From the predictive point of view, both CV and information criteria have three problems. The first is a theoretical problem about consistency. Both CV and information criteria are asymptotically unbiased estimators of the average generalization loss, in other words, their expectation values are asymptotically equal to that of the generalization loss. However, in general, the minimum point of a random function is not equal to that of the average function. Therefore, it has been unknown whether minimization of CV or information criteria is asymptotically equal to minimization of the average generalization loss or not. In this paper, we prove that, if a statistical model is regular, minimization of CV or WAIC makes the average generalization loss to be minimized asymptotically, whereas minimization of DIC or maximization of the marginal likelihood does not even asymptotically.

The second is a problem about the difference between the random and average generalization losses. The former is the random variable which depends on a given set of training samples, whereas the latter is the expectation value over all training sets taken from the true distribution. We show in this paper that the hyperparameter that minimizes the random generalization loss does not converge to that of the average generalization loss. It follows that, although the optimal hyperparameter for the minimum CV or WAIC asymptotically minimizes the average generalization loss, it does not the random generalization loss.

The last is a practical problem. When CV or information criteria is employed, it is not easy to determine the region of candidate hyperparameters, because we do not know whether the optimal hyperparameter exists, or, if it does, where it is. Moreover, after the region is determined, in order to compare CV or information criteria the posterior distributions are required for all candidate hyperparameters, resulting in heavy computational costs. The new formula obtained in this paper enables us to directly estimate CV and WAIC as a function of a hyperparameter, hence the optimal hyperparameter can be found without comparing candidate hyperparameters. Also we show a method by which the variances of the chosen hyperparameters by CV and WAIC are made smaller using the new formula.

This paper consists of eight sections. In the second and third sections, we define the basic definitions in Bayesian statistical learning and introduce the main results of this paper. In the fourth section, we study two examples. The fifth and sixth chapters are
devoted to the proofs of the basic lemmas and the main theorems respectively. In the seventh section, several points of the main results are discussed, and in the last section, we conclude the paper with the problem for the future study.

2 Basic Definitions in Bayesian Statistical Learning

In this section, we introduce the basic definitions in Bayesian statistical learning. Let \( q(x) \) be a probability density function on the \( N \) dimensional real Euclidean space \( \mathbb{R}^N \), and \( X_1, X_2, ..., X_n \) be random variables on \( \mathbb{R}^N \) which are independently subject to \( q(x) \). The probability density function \( q(x) \) is sometimes referred to as a true distribution. A training set is denoted by \( X^n = (X_1, X_2, ..., X_n) \), where \( n \) is the number of training samples. The average \( \mathbb{E}[\cdot] \) shows the expectation value overall training sets \( X^n \). A statistical model or a learning machine is defined by \( p(x|w) \) which is a probability density function of \( x \in \mathbb{R}^N \) for a given parameter \( w \in W \subseteq \mathbb{R}^d \). A nonnegative function \( \phi(w) \) on the parameter set \( W \) is called a prior distribution. If it satisfies

\[
\int \phi(w) dw = 1,
\]

then \( \phi(w) \) is called to be proper. In this paper, we study both proper and improper priors, hence eq. (1) does not hold in general. The posterior distribution is defined by

\[
p(w|X^n) = \frac{1}{Z(\phi)} \phi(w) \prod_{i=1}^{n} p(X_i|w),
\]

where \( Z(\phi) \) is a normalizing constant.

\[
Z(\phi) = \int \phi(w) \prod_{i=1}^{n} p(X_i|w) dw.
\]

We assume that \( Z(\phi) \) is finite with probability one. If \( \phi(w) \) is proper, then \( Z(\phi) \) is equal to the marginal likelihood. The expectation value of a given function \( f(w) \) over the posterior distribution is denoted by

\[
\mathbb{E}_\phi[f(w)] = \int f(w) p(w|X^n) dw.
\]

The predictive distribution is the average of a statistical model over the posterior distribution,

\[
p(x|X^n) = \mathbb{E}_\phi[p(x|w)].
\]

The random generalization loss is defined by

\[
G(\phi) = - \int q(x) \log p(x|X^n) dx.
\]

Note that the random variable \( G(\phi) \) depends on the training set \( X^n \). The average generalization loss is defined by \( \mathbb{E}[G(\phi)] \). In this paper, we show that the random variable
\( G(\varphi) \) has a different behavior from its expectation value \( \mathbb{E}[G(\varphi)] \) as a functional of \( \varphi(w) \) even asymptotically. The Bayesian leave-one-out cross validation (CV) is defined by

\[
\text{CV}(\varphi) = -\frac{1}{n} \sum_{i=1}^{n} \log p(X_i|X^n \setminus X_i)
\]

\[
= -\frac{1}{n} \sum_{i=1}^{n} \log \mathbb{E}_\varphi \left[ \frac{1}{p(X_i|w)} \right],
\]  

where \( X^n \setminus X_i \) is a set of training samples leaving \( X_i \) out. A calculation method of CV by eq.(7) using the posterior distribution by the Markov chain Monte Carlo method is sometimes called the important sampling cross validation. The training error \( T(\varphi) \) and the functional variance \( V(\varphi) \) are respectively defined by

\[
T(\varphi) = -\frac{1}{n} \sum_{i=1}^{n} \log p(X_i|X^n) = -\frac{1}{n} \sum_{i=1}^{n} \log \mathbb{E}_\varphi [p(X_i|w)],
\]

\[
V(\varphi) = \sum_{i=1}^{n} \{ \mathbb{E}_\varphi [(\log p(X_i|w))^2] - \mathbb{E}_\varphi [\log p(X_i|w)]^2 \}. 
\]

Then the widely applicable information criterion (WAIC) is defined by

\[
\text{WAIC}(\varphi) = T(\varphi) + \frac{1}{n} V(\varphi).
\]

For a real number \( \alpha \), the functional cumulant function is defined by

\[
F_{\text{cum}}(\alpha) = \frac{1}{n} \sum_{i=1}^{n} \log \mathbb{E}_\varphi [p(X_i|w)^\alpha].
\]

Then, as is shown in [Watanabe, 2010a],

\[
\text{CV}(\varphi) = F(-1),
\]

\[
T(\varphi) = -F(1),
\]

\[
V(\varphi) = nF''(0),
\]

\[
\text{WAIC}(\varphi) = -F(1) + F''(0).
\]

In the previous papers, we proved by singular learning theory that, even if a true distribution is unrealizable by a statistical model or even if the posterior distribution is not the normal distribution,

\[
\mathbb{E}[\text{CV}(\varphi)] = \mathbb{E}[G(\varphi)] + O(\frac{1}{n^2}),
\]

\[
\mathbb{E}[\text{WAIC}(\varphi)] = \mathbb{E}[G(\varphi)] + O(\frac{1}{n^2}),
\]

\[
\text{WAIC}(\varphi) = \text{CV}(\varphi) + O_p(\frac{1}{n^2}).
\]

However, it has been left unknown whether minimization of CV(\( \varphi \)) or WAIC(\( \varphi \)) with respect to a prior \( \varphi \) is asymptotically equivalent to minimization of \( G(\varphi) \) and \( \mathbb{E}[G(\varphi)] \) or not. In this paper, we prove in Theorem 1 that, if a statistical model satisfies the several
regularity conditions, minimization of CV(ϕ) or WAIC(ϕ) is asymptotically equivalent to minimization of E[G(ϕ)] but not to G(ϕ).

In the hyperparameter optimization problem, two alternative methods are well known. The former is maximization of the marginal likelihood or equivalently minimization of the free energy or the minus log marginal likelihood,

\[ F_{\text{free}}(\varphi) = -\log \int \varphi(w) \prod_{i=1}^{n} p(X_i|w) dw + \log \int \varphi(w) dw. \]  

(16)

In order to use this method, the integration of \( \varphi(w) \) should be finite, because, if it is not finite, \( F_{\text{free}}(\varphi) \) can not be defined. The latter is the deviance information criterion (DIC),

\[ \text{DIC}(\varphi) = \frac{1}{n} \sum_{i=1}^{n} \{-2E[\varphi][\log p(X_i|w)] + \log p(X_i|E[\varphi])\}. \]  

(17)

In this method a prior may be improper like as CV and WAIC. In this paper, we show that the hyperparameter which minimizes \( F_{\text{free}}(\varphi) \) or DIC(\( \varphi \)) does not minimize either \( E[G(\varphi)] \) or \( G(\varphi) \) even asymptotically in general.

3 Main Results

3.1 Definitions and Conditions

In this section, we introduce several notations, regularity conditions, and definitions of mathematical relations between priors.

The set of parameters \( W \) is assumed to be an open subset of \( \mathbb{R}^d \). In this paper, \( \varphi_0(w) \) is an arbitrary fixed prior and \( \varphi(w) \) is a candidate prior which will be optimized. We assume that, for an arbitrary \( w \in W \), \( \varphi_0(w) > 0 \) and \( \varphi(w) > 0 \). We do not assume that they are proper. The main purpose of this paper is make a new formula which enables us to directly estimate \( \text{CV}(\varphi) - \text{CV}(\varphi_0) \) and \( \text{WAIC}(\varphi) - \text{WAIC}(\varphi_0) \).

The prior ratio function \( \phi(w) \) is denoted by

\[ \phi(w) = \frac{\varphi(w)}{\varphi_0(w)}. \]

If \( \varphi_0(w) \equiv 1 \), then \( \phi(w) = \varphi(w) \). The empirical log loss function and the maximum a posteriori (MAP) estimator \( \hat{w} \) are respectively defined by

\[ L(w) = -\frac{1}{n} \sum_{i=1}^{n} \log p(X_i|w) - \frac{1}{n} \log \varphi_0(w), \]  

(18)

\[ \hat{w} = \arg \min_{w \in W} L(w), \]  

(19)

where either \( L(w) \) or \( \hat{w} \) does not depend on \( \varphi(w) \). If \( \varphi_0(w) \equiv 1 \), then \( \hat{w} \) is equal to the maximum likelihood estimator (MLE). The average log loss function and the parameter that minimizes it are respectively defined by

\[ \mathcal{L}(w) = -\int q(x) \log p(x|w) dx, \]  

(20)

\[ w_0 = \arg \min_{w \in W} \mathcal{L}(w). \]  

(21)
In this paper we use the following notations for simple description.

**Notations.**
(1) A parameter is denoted by \( w = (w^1, w^2, ..., w^k, ..., w^d) \in \mathbb{R}^d \). Remark that \( w^k \) means the \( k \)th element of \( w \), which does not mean \( w \) to the power of \( k \).
(2) For a given real function \( f(w) \) and nonnegative integers \( k_1, k_2, ..., k_m \), we define
\[
f_{k_1k_2...k_m} = f_{k_1k_2...k_m}(w) = \frac{\partial^m f}{\partial w^{k_1} \partial w^{k_2} ... \partial w^{k_m}}(w). \tag{22}
\]
(3) We adopt Einstein’s summation convention and \( k_1, k_2, k_3, ... \) are used for such suffices. For example,
\[
X_{k_1k_2} Y^{k_2k_3} = \sum_{k_2=1}^{d} X_{k_1k_2} Y^{k_2k_3}.
\]
In other words, if a suffix \( k_i \) appears both upper and lower, it means automatic summation over \( k_i = 1, 2, ..., d \). In this paper, for each \( k_1, k_2 \), \( X^{k_1k_2} = X_{k_1}^{k_2} = X_{k_2}^{k_1} \).

In order to prove the main theorem, we need the regularity conditions. In this paper, we do not study singular learning machines.

**Regularity Conditions.**
(1) *(Parameter Set)* The parameter set \( W \) is an open set in \( \mathbb{R}^d \).
(2) *(Smoothness of Models)* The functions \( \log \varphi(w) \), \( \log \varphi_0(w) \), and \( \log p(x|w) \) are \( C^\infty \) -class functions of \( w \in W \), in other words, they are infinitely many times differentiable.
(3) *(Identifiability of Parameter)* There exists a unique \( w_0 \in W \) which minimizes the average log loss function \( L(w) \). There exists a unique \( \hat{w} \in W \) which minimizes \( L(w) \) with probability one. It is assumed that the convergence in probability \( \hat{w} \to w_0 \) holds.
(4) *(Regularity Condition)* The matrix \( L_{k_1k_2}(w_0) \) is invertible. Also the matrix \( L_{k_1k_2}(w) \) is invertible for almost all \( w \) in a neighborhood of \( w_0 \) with probability one. Let \( J^{k_1k_2}(w) \) be the inverse matrix of \( L_{k_1k_2}(w) \).
(5) *(Well-Definedness and Concentration of Posterior)* We assume that, for an arbitrary \( |\alpha| \leq 1 \) and \( j = 1, 2, ..., n + 1 \),
\[
\mathbb{E}_{X_{n+1}} \mathbb{E} \left[ \log p(X_j|w)^\alpha \right] < \infty. \tag{23}
\]
The same inequality as eq. \((23)\) holds for \( \varphi_0(w) \) instead of \( \varphi(w) \). Let \( Q(X^n, w) \) be an arbitrary finite times product of
\[
\frac{1}{n} \sum_{i=1}^{n} \Pi (\log p(X_i|w))_{k_1k_2...k_r},
\]
where \( |\alpha| \leq 1 \), \( p, q, r, s \geq 0 \) and \( \Pi \) shows a finite product of a combination \( (k_1, k_2, ..., k_r) \). Let
\[
W(\varepsilon) = \{ w \in W ; |w - \hat{w}| < n^{\varepsilon - 1/2} \}. \tag{24}
\]
It is assumed that there exists $\varepsilon > 0$, for an arbitrary such product $Q(X^n, w)$,

$$
\mathbb{E}[\sup_{W(\varepsilon)} |Q(X^n, w)|] < \infty, \quad (25)
$$

$$
\mathbb{E}[Q(X^n, \hat{w})] \to \mathbb{E}[Q(X^n, w_0)], \quad (26)
$$

and that, for arbitrary $|\alpha| \leq 1$ and $\beta > 0$,

$$
\frac{\mathbb{E}_\varphi [Q(X^n, w)p(X_j|w)^\alpha]}{\mathbb{E}_\varphi [p(X_j|w)^\alpha]} = \left(1 + o_p\left(\frac{1}{n^\beta}\right)\right) \frac{\int_{W(\varepsilon)} Q(X^n, w)p(X_j|w)^\alpha \prod_{i=1}^n p(X_i|w)\varphi(w)dw}{\int_{W(\varepsilon)} p(X_j|w)^\alpha \prod_{i=1}^n p(X_i|w)\varphi(w)dw}, \quad (27)
$$

where $o_p(1/n^\beta)$ satisfies $n^\beta \mathbb{E}[|o_p(1/n^\beta)|] \to 0$. Also we assume that the same equation as eq.(27) holds for $\varphi_0(w)$ instead of $\varphi(w)$.

**Explanation of Regularity Condition.** (1) In this paper, we assume that $p(x|w)$ is regular at $w_0$, that is to say, the second order matrix $L_{k_1k_2}(w_0)$ is positive definite. If this condition is not satisfied, then such $(q(x), p(x|w))$ is called singular. The results of this paper do not hold for singular learning machines.

(2) Conditions eq.(25) and eq.(26) ensure the finiteness of the expectation values and concentration of the posterior distribution. The condition of the concentration, eq.(27), is set by the following mathematical reason. Let $S(w)$ be a function which takes the minimum value $S(\hat{w}) = 0$ at $w = \hat{w}$. If $S_{k_1k_2}(\hat{w})$ is positive definite, then by using the saddle point approximation in the neighborhood of $\hat{w}$,

$$
\exp(-nS(w)) \approx \exp\left(-\frac{n}{2}S_{k_1k_2}(\hat{w})(w - \hat{w})^{k_1}(w - \hat{w})^{k_2}\right),
$$

hence the orders of integrations inside and outside of $W(\varepsilon)$ are respectively given by

$$
\int_{W(\varepsilon)} \exp(-nS(w))dw = O(1/n^{d/2}),
$$

$$
\int_{W \setminus W(\varepsilon)} \exp(-nS(w))dw = O(\exp(-n^\varepsilon)).
$$

Therefore the integration over $W \setminus W(\varepsilon)$ converges to zero faster than that over $W(\varepsilon)$ as $n \to \infty$.

**Definition.** (Empirical Mathematical Relations between Priors) The empirical mathematical relation between two priors $\varphi(w)$ and $\varphi_0(w)$ at a parameter $w$ is defined by

$$
M(\phi, w) = A^{k_1k_2}(\log \phi)_{k_1}(\log \phi)_{k_2} + B^{k_1k_2}(\log \phi)_{k_1k_2} + C^{k_1}(\log \phi)_{k_1}, \quad (28)
$$
where \( \phi(w) = \varphi(w)/\varphi_0(w) \) and

\[
\begin{align*}
J^{k_1k_2}(w) &= \text{Inverse matrix of } L_{k_1k_2}(w), \\
A^{k_1k_2}(w) &= \frac{1}{2} J^{k_1k_2}(w), \\
B^{k_1k_2}(w) &= \frac{1}{2} (J^{k_1k_2}(w) + J^{k_1k_3}(w) J^{k_2k_1}(w) F_{k_3k_4}(w)), \\
C^{k_1}(w) &= J^{k_1k_2}(w) J^{k_2k_3}(w) F_{k_2k_4k_5}(w) - \frac{1}{2} J^{k_1k_2}(w) J^{k_2k_3}(w) L_{k_2k_3k_4}(w), \\
&\quad - \frac{1}{2} J^{k_1k_2}(w) J^{k_2k_3}(w) J^{k_5k_6}(w) L_{k_2k_3k_4}(w) F_{k_4,k_5,w}(w),
\end{align*}
\]

where \( L_{k_1k_2}(w) \) and \( L_{k_1k_2k_3}(w) \) are the second and third derivatives of \( L(w) \) respectively as defined by eq. (22) and

\[
F_{k_1,k_2}(w) = \frac{1}{n} \sum_{i=1}^{n} (\log p(X_i|w))_{k_1} (\log p(X_i|w))_{k_2}, \\
F_{k_1k_2,k_3}(w) = \frac{1}{n} \sum_{i=1}^{n} (\log p(X_i|w))_{k_1k_2} (\log p(X_i|w))_{k_3},
\]

**Remark.** Note that neither \( A^{k_1k_2}(w), B^{k_1k_2}(w), \) nor \( C^{k_1}(w) \) depends on a candidate prior \( \varphi(w) \).

**Definition.** (Average Mathematical Relations between Priors) The average mathematical relation \( M(\phi, w) \) is defined by the same manner as eq. (28) by using

\[
\begin{align*}
J^{k_1k_2}(w) &= \text{Inverse matrix of } L_{k_1k_2}(w), \\
L_{k_1k_2}(w) &= \int (-\log p(x|w))_{k_1k_2} q(x) dx, \\
L_{k_1k_2k_3}(w) &= \int (-\log p(x|w))_{k_1k_2k_3} q(x) dx, \\
F_{k_1,k_2}(w) &= \int (\log p(x|w))_{k_1} (\log p(x|w))_{k_2} q(x) dx, \\
F_{k_1k_2,k_3}(w) &= \int (\log p(x|w))_{k_1k_2} (\log p(x|w))_{k_3} q(x) dx,
\end{align*}
\]

instead of \( J^{k_1k_2}(w), L_{k_1k_2}(w), L_{k_1k_2k_3}(w), F_{k_1,k_2}(w), \) and \( F_{k_1k_2,k_3}(w) \) respectively.

The self-average mathematical relation \( \langle M \rangle(\phi, w) \) is defined by the same manner as \( M(\phi, w) \) by using

\[
\begin{align*}
\langle J^{k_1k_2} \rangle(w) &= \text{Inverse matrix of } \langle L_{k_1k_2} \rangle(w), \\
\langle L_{k_1k_2} \rangle(w) &= \int (-\log p(x|w))_{k_1k_2} p(x|w) dx, \\
\langle L_{k_1k_2k_3} \rangle(w) &= \int (-\log p(x|w))_{k_1k_2k_3} p(x|w) dx, \\
\langle F_{k_1,k_2} \rangle(w) &= \int (\log p(x|w))_{k_1} (\log p(x|w))_{k_2} p(x|w) dx, \\
\langle F_{k_1k_2,k_3} \rangle(w) &= \int (\log p(x|w))_{k_1k_2} (\log p(x|w))_{k_3} p(x|w) dx,
\end{align*}
\]

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instead of $J^{k_1k_2}(w)$, $L_{k_1k_2}(w)$, $L_{k_1k_2k_3}(w)$, $F_{k_1k_3}(w)$, and $F_{k_1k_2k_3}(w)$ respectively.

**Remark.** In the self-average case, it holds that $\langle L_{k_1k_2}(w) \rangle = \langle F_{k_1k_2}(w) \rangle$, hence $\langle M \rangle(\phi, w)$ can be calculated by the same manner as eq. (28) by using

\[
\langle A^{k_1k_2} \rangle(w) = \frac{1}{2} \langle J^{k_1k_2} \rangle(w),
\]

\[
\langle B^{k_1k_2} \rangle(w) = \langle J^{k_1k_2} \rangle(w),
\]

\[
\langle C^{k_1} \rangle(w) = \langle J^{k_1k_2} \rangle(w) \langle J^{k_3k_4} \rangle(w) - \langle J^{k_1k_2} \rangle(w) \langle J^{k_3k_4} \rangle(w) \langle L_{k_2k_3k_4} \rangle (w).
\]

instead of $A^{k_1k_2}(w)$, $B^{k_1k_2}(w)$ and $C^{k_1}(w)$.

### 3.2 Main Theorem

The following is the main result of this paper.

**Theorem 1.** Assume the regularity conditions (1), (2), ..., and (5). Let $M(\phi, w)$ and $\mathcal{M}(\phi, w)$ be the empirical and average mathematical relations between $\varphi(w)$ and $\varphi_0(w)$. Then

\[
\begin{align*}
\text{CV}(\varphi) &= \text{CV}(\varphi_0) + \frac{M(\phi, \hat{w})}{n^2} + O_p(\frac{1}{n^3}), \quad (39) \\
E[\text{CV}(\varphi)] &= E[\text{CV}(\varphi_0)] + \frac{M(\phi, w_0)}{n^2} + O(\frac{1}{n^3}), \quad (40) \\
\text{WAIC}(\varphi) &= \text{WAIC}(\varphi_0) + \frac{M(\phi, \hat{w})}{n^2} + O_p(\frac{1}{n^3}), \quad (41) \\
E[\text{WAIC}(\varphi)] &= E[\text{WAIC}(\varphi_0)] + \frac{M(\phi, w_0)}{n^2} + O(\frac{1}{n^3}), \quad (42) \\
\text{CV}(\varphi) &= \text{WAIC}(\varphi) + O_p(\frac{1}{n^2}), \quad (43)
\end{align*}
\]

and

\[
\begin{align*}
M(\phi, \hat{w}) &= M(\phi, w_0) + O_p(\frac{1}{n^{1/2}}), \quad (44) \\
M(\phi, E_w[w]) &= M(\phi, \hat{w}) + O_p(\frac{1}{n}), \quad (45) \\
E[M(\phi, \hat{w})] &= M(\phi, w_0) + O(\frac{1}{n}). \quad (46)
\end{align*}
\]

On the other hand,

\[
\begin{align*}
G(\varphi) &= G(\varphi_0) + \frac{1}{n}(\hat{w}^{k_1} - (w_0)^{k_1})(\log \phi)_{k_1}(\hat{w}) + O_p(\frac{1}{n^2}) \quad (47) \\
E[G(\varphi)] &= E[G(\varphi_0)] + \frac{M(\phi, w_0)}{n^2} + O(\frac{1}{n^3}). \quad (48)
\end{align*}
\]

From Theorem 1, the five mathematical facts are derived.

(1) Assume that a prior $\varphi(w)$ has a hyperparameter. Let $h(f)$ be the hyperparameter that minimizes $f(\varphi)$. By eq. (39) and eq. (41), $h(\text{CV})$ and $h(\text{WAIC})$ can be directly found by
minimizing the empirical mathematical relation \( M(\phi, \hat{w}) \) asymptotically. By eq.(44) and eq.(48), \( h(CV) \) and \( h(WAIC) \) is asymptotically equal to \( h(E[G]) \). Remark that \( CV(\varphi) \), \( WAIC(\varphi) \), and \( G(\varphi) \) may be unbounded or may not have a minimum value as a function of a hyperparameter if the set of all hyperparameters is not compact. By using \( M(\phi, \hat{w}) \), we can examine whether they have a minimum value or not. The divergence phenomenon of \( CV(\varphi) \) and \( WAIC(\varphi) \) as functions on a noncompact set of hyperparameters is discussed in Section 7.2.

2. The variance of \( h(CV) \) is asymptotically equal to that of \( h(WAIC) \), however, they may be different when the number of training samples are finite.

3. In calculation of the mathematical relation \( M(\phi, \hat{w}) \), the MAP estimator \( \hat{w} \) can be replaced by the posterior average parameter \( E[w] \) asymptotically.

4. By eq.(47), the variance of the random generalization loss \( G(\varphi) - G(\varphi_0) \) is larger than those of \( CV(\varphi_0) - CV(\varphi_0) \) and \( WAIC(\varphi_0) - WAIC(\varphi_0) \). Neither \( h(CV) \) nor \( h(WAIC) \) minimizes the random generalization loss \( G(\varphi) \) in general.

5. It was proved in (Watanabe, 2010) that \( E[G(\varphi_0)] = d/(2n) + o(1/n) \), where \( d \) is the dimension of the parameter set. Assume that there exist finite sets of real values \( \{d_k\} \) and \( \{\gamma_k\} \), where \( \gamma_k > 1 \), such that

\[
E[G(\varphi_0)] = \frac{d}{2n} + \sum_k \frac{d_k}{n^{\gamma_k}} + o(\frac{1}{n^2}).
\]

Since \( E[CV(\varphi_0)] \) of \( X^n \) is equal to \( E[G(\varphi_0)] \) of \( X^{n-1} \) and

\[
\frac{1}{n-1} - \frac{1}{n} = \frac{1}{n^2} + o(\frac{1}{n^2}),
\]

it immediately follows from Theorem 1 that

\[
E[G(\varphi)] = E[G(\varphi_0)] + \frac{M(\phi, w_0)}{n^2} + o(\frac{1}{n^2}), \tag{49}
\]

\[
E[CV(\varphi)] = E[G(\varphi_0)] + \frac{d/2 + M(\phi, w_0)}{n^2} + o(\frac{1}{n^2}), \tag{50}
\]

\[
E[WAIC(\varphi)] = E[G(\varphi_0)] + \frac{d/2 + M(\phi, w_0)}{n^2} + o(\frac{1}{n^2}). \tag{51}
\]

**Theorem 2.** Assume the regularity conditions (1), (2), ..., and (5). If there exists a parameter \( w_0 \) such that \( q(x) = p(x|w_0) \), then

\[
\langle M \rangle(\phi, \hat{w}) = M(\phi, \hat{w}) + O_p(\frac{1}{\sqrt{n}}), \tag{52}
\]

\[
\langle M \rangle(\phi, \hat{w}) = M(\phi, w_0) + O_p(\frac{1}{\sqrt{n}}). \tag{53}
\]

By Theorem 2, if the true distribution is realizable by a statistical model or a learning machine, then the empirical mathematical relation can be replaced by its self-average. The variance of the self-average mathematical relation is often smaller the original one, hence the variance of the estimated hyperparameter by using the self-average is made smaller.

Based on Theorem 1 and 2, we define new information criteria for hyperparameter optimization, the widely applicable information criterion for a regular case and a regular
case using self-average,

\[
\text{WAICR} = \frac{M(\phi, \hat{w})}{n^2},
\]

\[
\text{WAICRS} = \frac{\langle M(\phi, \hat{w}) \rangle}{n^2},
\]

where \(\hat{w}\) can be replaced by \(E_{\phi_0}[w]\). The optimal hyperparameter for predictive prior design can be directly found by minimization of these criteria if they have the minimum points.

4 Examples

4.1 Normal Distribution

A simple but nontrivial example is a normal distribution whose mean and standard deviation are \((m, 1/s)\),

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

For a prior distribution, we study

\[
\varphi(m, s|\lambda, \mu, \epsilon) = \exp\left(-\frac{\lambda sm^2 + \epsilon s}{2}\right)s^\mu,
\]

where \((\lambda, \mu, \epsilon)\) is a set of hyperparameters. Note that the prior is improper in general. If \(\lambda > 0, \mu > -1/2\) and \(\epsilon > 0\), the prior can be made proper by

\[
\Phi(m, s|\lambda, \mu, \epsilon) = \frac{1}{C}\varphi(m, s|\lambda, \mu, \epsilon),
\]

where

\[
C = \sqrt{\frac{2\pi}{\lambda}}(\epsilon/2)^{-\mu-1/2}\Gamma(\mu + 1/2).
\]

We use a fixed prior as \(\varphi_0(m, s) \equiv 1\), then the empirical log loss function is given by

\[
L(m, s) = -\frac{1}{2} \log \frac{s}{2\pi} + \frac{s}{2n} \sum_{i=1}^{n} (X_i - m)^2.
\]

Let \(M_j = (1/n) \sum_{i=1}^{n} (X_i - \hat{m})^j\) \((j = 2, 3, 4)\). The MAP estimator is equal to the MLE \(\hat{w} = (\hat{m}, \hat{s})\), where \(\hat{s}^2 = 1/M_2\), resulting that

\[
A^{k_1k_2}(\hat{w}) = \begin{pmatrix} 1/(2\hat{s}) & 0 \\ 0 & \hat{s}^2 \end{pmatrix},
\]

\[
P^{k_1k_2}(\hat{w}) = \begin{pmatrix} 1/\hat{s} & -\hat{s}^2 M_3/2 \\ -\hat{s}^2 M_3/2 & (\hat{s}^2 + \hat{s}^4 M_4)/2 \end{pmatrix},
\]

\[
C^{k_1}(\hat{w}) = (0, \hat{s} + \hat{s}^3 M_4).
\]
Also the self-average mathematical relation is given by

\[
\langle A^{k_1k_2}(\hat{\omega}) \rangle = \begin{pmatrix} 0 \\ \hat{s}^2 \end{pmatrix},
\]
\[
\langle B^{k_1k_2}(\hat{\omega}) \rangle = 2\langle A^{k_1k_2}(\hat{\omega}) \rangle,
\]
\[
\langle C^{k_1}(\hat{\omega}) \rangle = (0, \hat{s}).
\]

The prior ratio function is \( \phi(w) = \varphi(w) \), hence the derivatives of the log prior ratio are

\[
(\log \phi)_1(\hat{w}) = -\lambda \hat{s} \hat{m},
\]
\[
(\log \phi)_2(\hat{w}) = -\lambda \hat{m}^2/2 + \mu/\hat{s} - \varepsilon/2,
\]
\[
(\log \phi)_{11}(\hat{w}) = -\lambda \hat{s},
\]
\[
(\log \phi)_{12}(\hat{w}) = -\lambda \hat{m},
\]
\[
(\log \phi)_{22}(\hat{w}) = -\mu/\hat{s}^2.
\]

Therefore, the empirical and self-average mathematical relations are respectively

\[
M(\phi, \hat{m}, \hat{s}) = \frac{1}{2} \lambda^2 \hat{s} \hat{m}^2 + (-\lambda \hat{s} \hat{m}^2/2 + \mu - \varepsilon \hat{s}/2)^2
\]
\[
+ (-\lambda \hat{s} \hat{m}^2/2 + \mu/2 - \varepsilon \hat{s}/2)(1 + \hat{s}^2 M_4) - \lambda + \lambda \hat{m} s^2 M_3,
\]
\[
\langle M \rangle(\phi, \hat{m}, \hat{s}) = \frac{1}{2} \lambda^2 \hat{s} \hat{m}^2 + (-\lambda \hat{s} \hat{m}^2/2 + \mu - \varepsilon \hat{s}/2)^2
\]
\[
+ 4(-\lambda \hat{s} \hat{m}^2/2 + \mu/2 - \varepsilon \hat{s}/2) - \lambda.
\]

When \( \lambda = \varepsilon = 0 \), \( M(\varphi, \hat{m}, \hat{s}) \) is minimized at \( \mu = -(1 + \hat{s}^2 M_4)/4 \), whereas \( \langle M \rangle(\phi, \hat{m}, \hat{s}) \) at \( \mu = -1 \).

In this model, we can derive the exact forms of CV, WAIC, DIC, and the free energy, hence we can compare the optimal hyperparameters for these criteria. Let

\[
Z_n(X, \alpha) = \int p(X|w)^\alpha \prod_{i=1}^{n} p(X_i|w) \varphi(w) dw.
\]

Then

\[
Z_n(X, \alpha) = \frac{1}{(2\pi)^{n/2}} \exp\left( -\frac{\log a(\alpha)}{2} - c(\alpha) \log d(\alpha) \right) \Gamma(c(\alpha)),
\]

where \( \Gamma(\ ) \) is the gamma function and

\[
a(\alpha) = \alpha + \lambda + n,
\]
\[
b_i(\alpha) = \alpha X + \sum_{j=1}^{n} X_j^2,
\]
\[
c(\alpha) = \mu + (\alpha + n + 1)/2,
\]
\[
d_i(\alpha) = (1/2)(\alpha X + \sum_{j=1}^{n} X_j^2 - b_i(\alpha)^2/a(\alpha) + \varepsilon).
\]
Table 1: Averages and Standard Errors of Criteria

|        | $\mu$ | $\Delta C$  | $\Delta W$ | WAICR | WAICRS | $\Delta D$ | $\Delta G$ |
|--------|-------|-------------|-------------|-------|--------|------------|------------|
| Average| -1    | -0.00194    | -0.00175    | -0.00147 | -0.00165 | 0.00332    | -0.00156   |
| STD    | -1    | 0.00101     | 0.00080     | 0.00062 | 0.00001 | 0.00001    | 0.01292    |
| Average| 1     | 0.00506     | 0.00489     | 0.00450 | 0.00467 | 0.00006    | 0.00445    |
| STD    | 1     | 0.00095     | 0.00076     | 0.00059 | 0.00004 | 0.00002    | 0.01250    |

All criteria can be calculated by using $Z(X, \alpha)$ by their definitions,

$$CV(\varphi) = -\frac{1}{n} \sum_{i=1}^{n}\{\log Z_n(0,0) - \log Z_n(X_i,-1)\},$$

$$WAIC(\varphi) = -\frac{1}{n} \sum_{i=1}^{n}\{\log Z_n(X_i,1) - \log Z_n(0,0) - \frac{\partial^2}{\partial \alpha^2}(\log Z_n(X_i,0))\},$$

$$DIC(\varphi) = -\frac{1}{n} \sum_{i=1}^{n}\{2 \frac{\partial}{\partial \alpha}(\log Z_n(X_i,0)) - \log p(X_i,\overline{m},\overline{s})\},$$

$$F_{free}(\varphi) = -\log Z_n(0,0) + \log Z_0(0,0),$$

where $\overline{m} = b(0)/a(0)$ and $\overline{s} = (2\mu + n + 1)/(\sum X_i^2 - b(0)^2/a(0) + \varepsilon)$.

A numerical experiment was conducted. A true distribution $q(x)$ was set as $N(1,1^2)$. We study a case $n = 25$. Ten thousands independent training sets were collected. A statistical model and a prior were defined by eq.(56) and eq.(57) respectively. The fixed prior was $\phi_0(w) \equiv 1$. We set $\lambda = \varepsilon = 0.01$, and studied the optimization problem of the hyperparameter $\mu$. Firstly, we compared averages and standard deviations of criteria. In Table 1, averages and standard deviations of

$$\Delta C = CV(\varphi) - CV(\varphi_0),$$

$$\Delta W = WAIC(\varphi) - WAIC(\varphi_0),$$

$$WAICR = M(\varphi, \hat{w})/n^2,$$

$$WAICRS = \langle M(\varphi, \hat{w})/n^2,$$

$$\Delta D = DIC(\varphi) - DIC(\varphi_0),$$

$$\Delta G = G(\varphi) - G(\varphi_0),$$

are shown for the two cases $\mu = \pm 1$. In this experiment, averages of $\Delta C$, $\Delta W$, WAICR, and WAICRS were almost equal to that of $\Delta G$, however that of $\Delta D$ was not. The standard deviations were

$$\sigma(\Delta G) >> \sigma(\Delta C) > \sigma(\Delta W) > \sigma(WAICR) > \sigma(WAICRS) \approx \sigma(\Delta DIC).$$

The standard deviation of $\Delta G$ was largest which is consistent to Theorem 1. Note that CV had the larger variance than WAIC. WAICRS gave the most precise result.

Secondly, we compared the distributions of the chosen hyperparameters by criteria. One hundred candidate hyper parameters in the interval $(-2.5, 2.5)$ were compared and the optimal hyperparameter for each criterion was chosen by minimization. Remark that the interval for the free energy was set as $(-0.5, 2.5)$ because the prior is proper if and
only if $\mu > -0.5$. In Table 2, averages (A), standard deviations (STD), and $A \pm 2STD$ of optimal hyperparameters are shown.

In this case, the optimal hyperparameter for the minimum generalization loss is almost equal to $(-1)$, whose prior is improper. By CV, WAIC, WAICR, WAICRS, the optimal hyperparameter was almost chosen, whereas by DIC or the free energy, it was not. The standard deviations of chosen hyperparameters were

$$\sigma(h(CV)) > \sigma(h(WAIC)) > \sigma(h(WAICR))$$

$$> \sigma(h(F)) > \sigma(h(DIC)) > \sigma(h(WAICRS)).$$

In this experiment, neither the marginal likelihood nor DIC was appropriate for the predictive prior design.

### 4.2 Linear Regression

Let us study a linear regression problem. Let a statistical model of $y \in \mathbb{R}^1$, $x \in \mathbb{R}^d$, $w \in \mathbb{R}^d$, and $\lambda \in \mathbb{R}^1$ be

$$p(y|x, w) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{1}{2\sigma^2}(y - w \cdot x)^2\right),$$

$$\varphi(w|\lambda) = \exp\left(-\frac{\lambda}{2}\|w\|^2\right),$$

where $\sigma > 0$ is a constant. The basic prior is set as $\varphi_0(w) \equiv 1$. Hence the log prior ratio function is $\phi(w) = \varphi(w|\lambda)$ and $\hat{w}$ is equal to MLE. The function $L(w)$ without a constant term is

$$L(w) = \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - w \cdot x_i)^2.$$
It is immediately derived that
\[
\hat{w}_{k_1} = \left( \sum_{i=1}^{n} x_{ik_1} x_{ik_2} \right)^{-1} \left( \sum_{i=1}^{n} y_{i} x_{ik_1} \right),
\]
(68)
\[
L_{k_1 k_2} (\hat{w}) = \frac{1}{\sigma^2 n} \sum_{i=1}^{n} x_{ik_1} x_{ik_2},
\]
(69)
\[
L_{k_1 k_2 k_3} (\hat{w}) = 0,
\]
(70)
\[
F_{k_1, k_2} (\hat{w}) = \frac{1}{\sigma^2 n} \sum_{i=1}^{n} (y_i - \hat{w} \cdot x_i)^2 x_{ik_1} x_{ik_2},
\]
(71)
\[
F_{k_1 k_2, k_3} (\hat{w}) = - \frac{1}{\sigma^2 n} \sum_{i=1}^{n} (y_i - \hat{w} \cdot x_i) x_{ik_1} x_{ik_2} x_{ik_3},
\]
(72)
\[
(\log \phi)_{k_1} (\hat{w}) = - \lambda \lambda_{k_1}, \quad (\log \phi)_{k_2} (\hat{w}) = - \lambda \lambda_{k_2},
\]
(73)
(74)
and \( J_{k_1 k_2} (\hat{w}) = (L_{k_1 k_2})^{-1} (\hat{w}) \). Hence
\[
A^{k_1 k_2} (\hat{w}) = \frac{1}{2} J_{k_1 k_2} (\hat{w}),
\]
(75)
\[
B^{k_1 k_2} (\hat{w}) = \frac{1}{2} \{ J_{k_1 k_2} (\hat{w}) + J^{k_1 k_3} (\hat{w}) J^{k_2 k_4} (\hat{w}) F_{k_3 k_4} (\hat{w}) \},
\]
(76)
\[
C^{k_1} (\hat{w}) = J^{k_1 k_2} (\hat{w}) J^{k_3 k_4} (\hat{w}) F_{k_2 k_3 k_4} (\hat{w}),
\]
(77)
resulting that
\[
M (\phi, \hat{w}) = \frac{\lambda^2}{2} (J^{k_1 k_2} (\hat{w}) \hat{w}_{k_1} \hat{w}_{k_2}) - \lambda \text{tr} (B (\hat{w}) + C^{k_1} (\hat{w}) \hat{w}_{k_1}),
\]
(78)
\[
\langle M \rangle (\phi, \hat{w}) = \frac{\lambda^2}{2} (J^{k_1 k_2} (\hat{w}) \hat{w}_{k_1} \hat{w}_{k_2}) - \lambda \text{tr} (J (\hat{w})),
\]
(79)
where we used \( \langle B \rangle^{k_1 k_2} = J^{k_1 k_2} \) and \( \langle C \rangle^{k_1} (\hat{w}) = 0 \). In this model the optimal hyperparameter for WAICRS is directly given by
\[
\lambda = \frac{\text{tr} (J (\hat{w}))}{J^{k_1 k_2} (\hat{w}) \hat{w}_{k_1} \hat{w}_{k_2}}.
\]
(80)
The exact CV, WAIC, DIC, and the free energy are also calculated. Let
\[
Z_n (X, Y, \alpha) = \int p(Y | X, w)^{\alpha} \prod_{i=1}^{n} p(Y_i | X_i, w) \varphi (w) dw.
\]
Then
\[
Z_n (X, Y, \alpha) = \frac{(\lambda \sigma^2)^{d/2} \exp \left( \frac{1}{2 \sigma^2} \{ b(\alpha)^T A(\alpha)^{-1} b(\alpha) - (\alpha Y^2 + \sum_{i=1}^{n} Y_i^2) \} \right)}{(2 \pi \sigma^2)^{(n+\alpha)/2} \det (A(\alpha))^{1/2}},
\]
where
\[
A(\alpha) = \alpha XX^T + \sigma^2 \lambda I + \sum_{i=1}^{n} X_i X_i^T,
\]
\[
b(\alpha) = \alpha Y X + \sum_{i=1}^{n} Y_i X_i.
\]
|          | h(CV)  | h(WAIC) | h(WAICR) | h(WAICRS) | h(DIC)  | h(F)   |
|----------|--------|---------|----------|-----------|---------|--------|
| Average  | 5.0064 | 5.0017  | 4.9320   | 5.0253    | 5.0248  | 1.0000 |
| STD      | 1.9358 | 1.9297  | 1.8808   | 0.2960    | 0.2961  | 0.0000 |

Table 3: Chosen Hyperparameters in linear regression

All criteria can be calculated by using $Z(X, Y, \alpha)$ by their definitions,

$$CV(\varphi) = -\frac{1}{n} \sum_{i=1}^{n} \{ \log Z_n(0, 0, 0) - \log Z_n(X_i, Y_i, -1) \},$$

$$WAIC(\varphi) = -\frac{1}{n} \sum_{i=1}^{n} \{ \log Z_n(X_i, Y_i, 1) - \log Z_n(0, 0, 0) - \frac{\partial^2}{\partial \alpha^2} (\log Z_n(X_i, Y_i, 0)) \},$$

$$DIC(\varphi) = -\frac{1}{n} \sum_{i=1}^{n} \{ 2 \frac{\partial}{\partial \alpha} (\log Z_n(X_i, 0, 0)) - \log p(X_i, Y_i, \bar{m}) \},$$

$$F_{free}(\varphi) = -\log Z_n(0, 0, 0) + \log Z_n(0, 0, 0),$$

where $\bar{m} = A(0)^{-1} b(0)$.

A numerical experiment was conducted for the case $q(x, y) = q(x)p(y|x, w_0)$. Here $q(x)$ was the normal distribution $N(a_0, I_5)$, where $a_0 = (1, 1, 1, 1, 1)$, and $I_5$ is the $d = 5$ dimensional identity matrix, and $w_0 = (1, 1, 1, 1, 1)$. A constant $\sigma = 0.1$ was set. The candidate hyperparameters for $\lambda$ were taken from the interval $(0, 10)$. Distributions of chosen hyperparameters are shown in Table 3. The average hyperparameters chosen by CV, WAIC, WAICR, WAICRS, and DIC were almost equal to each others. The variances by WAICRS and DIC were smaller than other methods. The optimal hyperparameter by the marginal likelihood was different from other methods. In this case, the posterior distribution is rigorously equal to the normal distribution and the true distribution is realizable by a statistical model, hence DIC can be applied, whose value was almost equal to WAICRS. Note that, in this model, the true parameter is $w_0 = 0$, then the optimal hyperparameter $\lambda$ diverges as $n \to \infty$. This phenomenon is caused by the fact that $w_0 = 0$ is contained in the divergent parameter, which is discussed in Section 7.2.

5 Basic Lemmas

The main purpose of this paper is to prove Theorems 1 and 2. In this section we prepare several lemmas which are used in the proof of the main theorem.

For arbitrary function $f(w)$, we define the expectation values by

$$E_{\varphi}^{(\pm j)}[f(w)] = \frac{\int f(w)\varphi(w)p(X_j|w)\pm^1 \prod_{i=1}^{n} p(X_i|w) dw}{\int \varphi(w)p(X_j|w)\pm^1 \prod_{i=1}^{n} p(X_i|w) dw}.$$

Then the predictive distribution of $x$ using training samples $X^n$ leaving $X_j$ out is

$$E_{\varphi}^{(-j)}[p(x|w)].$$
Thus its log loss for the test sample \( X_j \) is
\[
- \log \mathbb{E}_\phi^{(-j)}[p(X_j|w)].
\]
The log loss of the leave-one-out cross validation is then given by
\[
\text{CV}(\phi) = -\frac{1}{n} \sum_{j=1}^{n} \log \mathbb{E}_\phi^{(-j)}[p(X_j|w)]. \tag{81}
\]

**Lemma 1.** Let \( \phi(w) = \frac{\varphi(w)}{\varphi_0(w)} \). The cross validation and the generalization error satisfy the following equations.

\[
\text{CV}(\phi) = \text{CV}(\phi_0) + \frac{1}{n} \sum_{j=1}^{n} \{ \log \mathbb{E}_{\phi_0}^{(-j)}[\phi(w)] - \log \mathbb{E}_{\phi_0}[\phi(w)] \}, \tag{82}
\]

\[
G(\phi) = G(\phi_0) - \mathbb{E}_{X_{n+1}} \left[ \log \mathbb{E}_{\phi_0}^{(+{(n+1)})}[\phi(w)] - \log \mathbb{E}_{\phi_0}[\phi(w)] \right]. \tag{83}
\]

(Proof of Lemma 1) By the definitions \( \mathbb{E}_\phi[\cdot] \), \( \mathbb{E}_\phi^{(-j)}[\cdot] \), it follows that

\[
\mathbb{E}_{\phi}^{(-j)}[p(X_j|w)] = \frac{\int \varphi(w) \prod_{i=1}^{n} p(X_i|w)dw}{\int \varphi(w) \prod_{i \neq j}^{n} p(X_i|w)dw} = \frac{\int \varphi_0(w) \prod_{i=1}^{n} p(X_i|w)dw \int \varphi_0(w) \prod_{i \neq j}^{n} p(X_i|w)dw}{\int \varphi_0(w) \prod_{i=1}^{n} p(X_i|w)dw \int \varphi_0(w) \prod_{i \neq j}^{n} p(X_i|w)dw} \times \frac{\int \varphi_0(w) \prod_{i \neq j}^{n} p(X_i|w)dw}{\int \varphi_0(w) \prod_{i \neq j}^{n} p(X_i|w)dw} = \mathbb{E}_{\phi_0}[\phi] \mathbb{E}_{\phi_0}^{(-j)}[p(X_j|w)] / \mathbb{E}_{\phi_0}^{(-j)}[\phi].
\]

By the definition \( \text{CV}(\phi) \), eq. (81), the first half of Lemma 1 is obtained. For the latter
\[
\mathbb{E}_\phi[p(X_{n+1}|w)] = \frac{\int \varphi(w)p(X_{n+1}|w) \prod_{i=1}^{n} p(X_i|w) dw}{\int \varphi(w) \prod_{i=1}^{n} p(X_i|w) dw} = \frac{\int \varphi(w) \prod_{i=1}^{n+1} p(X_i|w) dw}{\int \varphi_0(w) \prod_{i=1}^{n+1} p(X_i|w) dw}
\]

By using the definition of the generalization error, eq.(5), the latter half of Lemma 1 is obtained. (Q.E.D.)

**Definition.** The log loss function for \(X^n \setminus X_j\) is defined by

\[
L(w, -j) = -\frac{1}{n} \sum_{i \neq j}^{n} \log p(X_i|w) - \frac{1}{n} \log \varphi_0(w).
\]

The MAP estimator for \(X^n \setminus X_j\) is denoted by

\[\hat{w}_j = \arg \min L(w, -j).\]

**Lemma 2.** Let \(f(w)\) be a function \(Q(X^n, w)\) which satisfies the regularity conditions (1), (2), ..., (5). Then there exist functions \(R_1(f, w)\) and \(R_2(f, w)\) which satisfy

\[
\mathbb{E}_\varphi_0[f(w)] = f(\hat{w}) + R_1(f, \hat{w}) + R_2(f, \hat{w}) + O_p\left(\frac{1}{n^3}\right), \quad (84)
\]

\[
\mathbb{E}_\varphi_0^{-j}[f(w)] = f(\hat{w}_j) + R_1(f, \hat{w}_j) + R_2(f, \hat{w}_j) + O_p\left(\frac{1}{n^3}\right), \quad (85)
\]

where \(R_1(f, w)\) is given by

\[
R_1(f, w) = \frac{1}{2} f_{k_1k_2}(w) J^{k_1k_2}(w) - \frac{1}{2} f_{k_1}(w) V^{k_1}(w), \quad (86)
\]

and \(V^{k_1}(w) = J^{k_1k_2}(w) J^{k_3k_4}(w) L_{k_2k_3k_4}(w).\)

We do not need the concrete form of \(R_2(f, w)\) in the proof of the main theorem. However, it is given in the proof of Lemma 2, eq.(108).
(Proof of Lemma 2) Since $L(\hat{w})$ is a constant function of $w$, by using the regularity condition (5),

\[
\mathbb{E}_{\varphi_0}[f(w)] = \frac{\int f(w) \exp(-nL(w) + nL(\hat{w}))dw}{\int \exp(-nL(w) + nL(\hat{w}))dw} = f(\hat{w}) + \frac{\int (f(w) - f(\hat{w})) \exp(-nL(w) + nL(\hat{w}))dw}{\int \exp(-nL(w) + nL(\hat{w}))dw} = f(\hat{w}) + \frac{Z_1}{Z_0}(1 + O_p\left(\frac{1}{n^\beta}\right)),
\]

(87)

where

\[
Z_1 = \int_{W(\varepsilon)} (f(w) - f(\hat{w})) \exp(-nL(w) + nL(\hat{w}))dw,
\]

(88)

\[
Z_0 = \int_{W(\varepsilon)} \exp(-nL(w) + nL(\hat{w}))dw.
\]

(89)

Note that the definition of $W(\varepsilon)$ is given in eq.(24). Let $u = \sqrt{n}(w - \hat{w})$. Then $du = n^{d/2}dw$ and the integrated region is $|u| < n^\varepsilon$. The Taylor expansions of $f(w)$ and $nL(w)$ among $\hat{w}$ are respectively given by

\[
f(w) - f(\hat{w}) = H_1(u),
\]

\[
n(L(w) - L(\hat{w})) = \frac{1}{2} L_{k_1 k_2} u^{k_1} u^{k_2} + H_2(u),
\]

where $H_1(u)$ and $H_2(u)$ are functions defined by

\[
H_1(u) = \frac{1}{n^{1/2}} f_{k_1} u^{k_1} + \frac{1}{2n} f_{k_1 k_2} u^{k_1} u^{k_2} + \frac{1}{6n^{3/2}} f_{k_1 k_2 k_3} u^{k_1} u^{k_2} u^{k_3}
+ \frac{1}{24n^2} f_{k_1 k_2 k_3 k_4} u^{k_1} u^{k_2} u^{k_3} u^{k_4} + \frac{g_1(u)}{n^{5/2}},
\]

(90)

\[
H_2(u) = \frac{1}{6n^{1/2}} L_{k_1 k_2 k_3} u^{k_1} u^{k_2} u^{k_3} + \frac{1}{24n} L_{k_1 k_2 k_3 k_4} u^{k_1} u^{k_2} u^{k_3} u^{k_4}
+ \frac{1}{120n^{3/2}} L_{k_1 k_2 k_3 k_4 k_5} u^{k_1} u^{k_2} u^{k_3} u^{k_4} u^{k_5} + \frac{g_2(u)}{n^2},
\]

(91)

where $g_1(u)$ and $g_2(u)$ are constant order functions. In these equations, the derivatives of $f$ and $L$ are defined by their values at $w = \hat{w}$. We use notations,

\[
\rho(u) = \exp\left(-\frac{1}{2} L_{k_1 k_2} u^{k_1} u^{k_2}\right),
\]

(92)

\[
c_0 = \int \rho(u)du = \frac{(2\pi)^{d/2}}{\det(L_{k_1 k_2})^{1/2}}.
\]

(93)
Remark that $J^{k_1k_2}$ is the inverse matrix of $L_{k_1k_2}$, hence
\[
\int u^{k_1}u^{k_2}\rho(u)du = c_0 J^{k_1k_2}, \tag{94}
\]
\[
\int \prod_{j=1}^{4} u^{k_j}\rho(u)du = c_0 \{ J^{k_1k_2}J^{k_3k_4} + J^{k_1k_3}J^{k_2k_4} + J^{k_1k_4}J^{k_2k_3} \}, \tag{95}
\]
\[
\int \prod_{j=1}^{6} u^{k_j}\rho(u)du = c_0 Sym(J)^{k_1k_2k_3k_4k_5k_6}, \tag{96}
\]
\[
\int \prod_{j=1}^{8} u^{k_j}\rho(u)du = c_0 Sym(J)^{k_1k_2k_3k_4k_5k_6k_7k_8}, \tag{97}
\]
where
\[
Sym(J)^{k_1k_2k_3k_4k_5k_6} = \sum_{m_1,...,m_6} J^{m_1m_2}J^{m_3m_4}J^{m_5m_6}, \tag{98}
\]
\[
Sym(J)^{k_1k_2k_3k_4k_5k_6k_7k_8} = \sum_{m_1,...,m_8} J^{m_1m_2}J^{m_3m_4}J^{m_5m_6}J^{m_7m_8}. \tag{99}
\]
Here $\sum_{m_1,...,m_6}$ is the sum of all 15 different pair combinations of $(k_1, ..., k_6)$ and $\sum_{m_1,...,m_8}$ is the sum of all 105 different pair combinations of $(k_1, ..., k_8)$. By using these results, $Z_0$ in eq. (89) is given by
\[
Z_0 = \frac{1}{n^{d/2}} \int_{|u|<n^c} \exp(-H_2(u))\rho(u)du
= \frac{1}{n^{d/2}} \int_{|u|<n^c} \left\{1 - H_2(u) + \frac{H_2(u)^2}{2} - \frac{H_2(u)^3}{6} + O_p(n^{-2}) \right\}\rho(u)du. \tag{100}
\]
Then by using the symmetry of the integrated region, the integrations of the odd order terms are equal to zero. It follows that
\[
Z_0 = \frac{c_0}{n^{d/2}} \left(1 + \frac{Y_1(\hat{w})}{n} + O_p\left(\frac{1}{n^2}\right)\right), \tag{101}
\]
where
\[
Y_1(\hat{w}) = \frac{1}{c_0} \int \left\{-\frac{1}{24}L_{k_1k_2k_3k_4}u^{k_1}u^{k_2}u^{k_3}u^{k_4} + \frac{1}{72}(L_{k_1k_2k_4}u^{k_1}u^{k_2}u^{k_3})^2\right\}\rho(u)du
= -\frac{1}{8}L_{k_1k_2k_3k_4}J^{k_1k_2}J^{k_3k_4} + \frac{5}{24}L_{k_1k_2k_3}L_{k_4k_5k_6}J^{k_1k_2}J^{k_3k_4}J^{k_5k_6}, \tag{102}
\]
where we used eq. (95) and eq. (96). On the other hand, $Z_1$ in eq. (88) is given by
\[
Z_1 = \frac{1}{n^{d/2}} \int_{|u|<n^c} H_1(u)\exp(-H_2(u))\rho(u)du
= \frac{1}{n^{d/2}} \int_{|u|<n^c} H_1(u)\left\{1 - H_2(u) + \frac{H_2(u)^2}{2} - \frac{H_2(u)^3}{6} + O_p(n^{-2}) \right\}\rho(u)du. \tag{103}
\]
Then by using symmetry of the integrated region, it follows that
\[
Z_1 = \frac{c_0}{n^{d/2}} \left(\frac{Y_2(\hat{w})}{n} + \frac{Y_3(\hat{w})}{n^2} + O_p\left(\frac{1}{n^2}\right)\right), \tag{104}
\]
where $Y_2(\hat{w})$ and $Y_3(\hat{w})$ are given by

\[
Y_2(\hat{w}) = \frac{1}{c_0} \int \left\{ \frac{1}{2} f_{k_1 k_2} u^{k_1} u^{k_2} - \frac{1}{6} f_{k_1} L_{k_2 k_3 k_4} u^{k_1} u^{k_2} u^{k_3} u^{k_4} \right\} \rho(u) \, du
\]

\[
= \frac{1}{2} f_{k_1 k_2} J^{k_1 k_2} - \frac{1}{2} f_{k_1} L_{k_2 k_3 k_4} J^{k_1 k_2} J^{k_3 k_4},
\]

(105)

\[
Y_3(\hat{w}) = \frac{1}{c_0} \int \rho(u) \, du \left\{ \frac{1}{24} f_{k_1 k_2 k_3 k_4} u^{k_1} u^{k_2} u^{k_3} u^{k_4}
\]

\[-\left( \frac{1}{120} f_{k_1} L_{k_2 k_3 k_4 k_5} + \frac{1}{48} f_{k_1 k_2} L_{k_3 k_4 k_5 k_6} + \frac{1}{36} f_{k_1 k_2 k_3} L_{k_4 k_5 k_6} \right) \prod_{j=1}^{6} \alpha^j
\]

\[+ \frac{1}{144} \left( f_{k_1} L_{k_2 k_3 k_4} L_{k_5 k_6 k_7 k_8} + f_{k_1 k_2} L_{k_3 k_4 k_5} L_{k_6 k_7 k_8} \right) \prod_{j=1}^{8} \alpha^j \}
\]

\[=
\frac{1}{8} f_{k_1 k_2 k_3 k_4} J^{k_1 k_2} J^{k_3 k_4} - \left( \frac{1}{120} f_{k_1} L_{k_2 k_3 k_4 k_5}
\right.
\]

\[+ \frac{1}{48} f_{k_1 k_2} L_{k_3 k_4 k_5} + \frac{1}{36} f_{k_1 k_2 k_3} L_{k_4 k_5 k_6} \right) \text{Sym}(J)^{k_1 k_2 k_3 k_4 k_5 k_6}
\]

\[+ \frac{1}{144} \left( f_{k_1 k_2} L_{k_2 k_3 k_4} L_{k_5 k_6 k_7 k_8} + f_{k_1 k_2 k_3} L_{k_4 k_5 k_6} \right) \text{Sym}(J)^{k_1 k_2 k_3 k_4 k_5 k_6 k_7 k_8},
\]

where we used eq. (95), eq. (96), and eq. (97). Summing up these results,

\[
E_{\phi_0}[f(w)] = f(\hat{w}) + \frac{Z_1}{Z_0} \left( 1 + O_p(\frac{1}{n^3}) \right)
\]

\[= f(\hat{w}) + \frac{Y_2(\hat{w})/n + Y_3(\hat{w})/n^2 + O_p(1/n^3)}{Y_1(\hat{w})/n + O_p(1/n^2)} \left( 1 + O_p(\frac{1}{n^3}) \right)
\]

\[= f(\hat{w}) + \frac{Y_2(\hat{w})/n + Y_3(\hat{w}) - Y_1(\hat{w}) Y_2(\hat{w})}{Y_1(\hat{w})/n + O_p(1/n^2)}. \quad (106)
\]

Therefore, by putting

\[
R_1(f, \hat{w}) = Y_2(\hat{w}),
\]

(107)

\[
R_2(f, \hat{w}) = Y_3(\hat{w}) - Y_1(\hat{w}) Y_2(\hat{w}),
\]

(108)

the first half of Lemma is completed. The latter half is equal to the case when the training samples are $X^n$ leaving $X_j$ out, hence it is immediately obtained from the first half. (Q.E.D.)

**Lemma 3.** Let $|\alpha| \leq 1$. If $m$ is a positive odd number,

\[
\frac{E_{\phi_0}[p(X_k|w)^\alpha \prod_{j=1}^{m} (w^{k_j} - \hat{w}^{k_j})]}{E_{\phi_0}[p(X_k|w)^\alpha]} = O_p(\frac{1}{n^{(m+1)/2}}).
\]

(109)

If $m$ is a positive even number,

\[
\frac{E_{\phi_0}[p(X_k|w)^\alpha \prod_{j=1}^{m} (w^{k_j} - \hat{w}^{k_j})]}{E_{\phi_0}[p(X_k|w)^\alpha]} = O_p(\frac{1}{n^{m/2}}).
\]

(110)

For $m = 2, 4$,

\[
E_{\phi_0}[\prod_{j=1}^{2} (w^{k_j} - \hat{w}^{k_j})] = \frac{1}{n} J^{k_1 k_2} + O_p(\frac{1}{n^2}),
\]

(111)

\[
E_{\phi_0}[\prod_{j=1}^{4} (w^{k_j} - \hat{w}^{k_j})] = \frac{1}{n^2} (J^{k_1 k_2} J^{k_3 k_4} + J^{k_1 k_3} J^{k_2 k_4} + J^{k_1 k_4} J^{k_2 k_3}) + O_p(\frac{1}{n^3}).
\]

(112)
(Proof of Lemma 3) In this proof, we use same notations as the proof of Lemma 2. By the regularity condition (5),

\[
\mathbb{E}_{\phi_0}[p(X_k|w)^\alpha \prod_{j=1}^m (w_j^{k_j} - \hat{w}_j^{k_j})] = \frac{Z_m^*}{Z_0} (1 + O_p(\frac{1}{n^\beta}))
\]

for an arbitrary \( \beta > 0 \), where

\[
Z_m^* = \int_{W(\epsilon)} \prod_{j=1}^m (w_j^{k_j} - \hat{w}_j^{k_j}) \exp(-nL(w) + nL(\hat{w}) + \alpha \eta(X_k, w)) dw
\]

\[
= \frac{1}{n^{(m+d)/2}} \int_{|u| < n^\epsilon} \prod_{j=1}^m u_j^{k_j} \exp(-H_2(u) + \alpha \eta(X_k, \hat{w} + u/\sqrt{n})) \rho(u) du. \tag{113}
\]

Here we used a notation, \( \eta(X_k, w) = \log p(X_k|w) - \log p(X_k|\hat{w}) \). By eq. (111), the first term of \( H_2(u) \) is in proportion to \( u^3/n^{1/2} \). Moreover, there exists \( u^* \) such that \( \eta(X_k, \hat{w} + u/\sqrt{n}) \). Hence by the expansion of

\[
\exp(-H_2(u) + \alpha \eta(X_k, u^*)/\sqrt{n}) = 1 + \{-H_2(u) + \alpha \eta(X_k, u^*)/\sqrt{n}\} + O_p(1/n),
\]

if \( m \) is an odd number, \( Z_m = O_p(1/n^{(m+d+1)/2}) \), which shows eq. (109), and if \( m \) is an even number, \( Z_m = O_p(1/n^{(m+d)/2}) \), which shows eq. (110). By using eq. (94) and eq. (95) in the case \( \alpha = 0 \), the results for \( m = 2, 4 \) are derived. (Q.E.D.)

**Definition.** We use several functions of \( w \) in the proof.

\[
S^{k_1}(w) = J^{k_1k_2}(w) J^{k_3k_4}(w) F_{k_2k_3k_4}(w), \tag{114}
\]

\[
T^{k_1}(w) = J^{k_1k_2}(w) J^{k_3k_5}(w) F_{k_2k_3k_5}(w), \tag{115}
\]

\[
U^{k_1k_2}(w) = J^{k_1k_3}(w) J^{k_4k_5}(w) F_{k_1k_4k_5}(w). \tag{116}
\]

**Lemma 4.** Let \( \hat{w} \) and \( \hat{w}_j \) be the MAP estimator for \( X^n \) and \( X^n \setminus X_j \), respectively. Then

\[
\frac{1}{n} \sum_{j=1}^n \{ (\hat{w}_j)^{k_1} - \hat{w}_j^{k_1} \} = \frac{1}{n^2} S^{k_1}(\hat{w}) - \frac{1}{2n} T^{k_1}(\hat{w}) + O_p(\frac{1}{n^3}), \tag{117}
\]

\[
\frac{1}{n} \sum_{j=1}^n \{(\hat{w}_j)^{k_1} - \hat{w}_j^{k_1}\} \{ (\hat{w}_j)^{k_2} - \hat{w}_j^{k_2}\} = \frac{1}{n^2} U^{k_1k_2}(\hat{w}) + O_p(\frac{1}{n^3}). \tag{118}
\]

For an arbitrary \( C^\infty \)-class function \( f(w) \)

\[
\frac{1}{n} \sum_{j=1}^n \{ f(\hat{w}_j) - f(\hat{w}) \} = \frac{1}{n^2} \{ f^{k_1}(\hat{w}) S^{k_1}(\hat{w}) - \frac{1}{2} T^{k_1}(\hat{w}) \}
\]

\[
+ \frac{1}{2} f^{k_1k_2}(\hat{w}) U^{k_1k_2}(\hat{w}) + O_p(\frac{1}{n^3}). \tag{119}
\]

(Proof of Lemma 4) In this proof, we use a notation, \( \ell(j, w) = \log p(X_j, w) \). Since \( \hat{w}_j \) minimizes \( L(w, \cdot) \), its derivative is equal to zero at \( \hat{w}_j \),

\[
L_{k_1}(\hat{w}_j, \cdot) = 0. \tag{120}
\]
By using the mean value theorem, there exists a parameter $w^*$ which satisfies $\|w^* - \hat{w}\| \leq \|\hat{w}_j - \hat{w}\|$ and

$$L_{k_1}(\hat{w}, -j) + L_{k_1 k_2}(w^*, -j)((\hat{w}_j)^{k_2} - \hat{w}^{k_2}) = 0. \quad (121)$$

Note that the MAP estimator $\hat{w}$ minimizes $L(w)$ where

$$L(w) = L(w, -j) - \frac{1}{n} \ell(j, w), \quad (122)$$

hence its derivative satisfies $L_{k_1}(\hat{w}) = 0$. Therefore

$$L_{k_1}(\hat{w}, -j) = \frac{1}{n} \ell_{k_1}(j, \hat{w}). \quad (123)$$

By applying eq. (123) to eq. (121),

$$(\hat{w}_j)^{k_1} - \hat{w}^{k_1} = -\frac{1}{n} (L(w^*, -j)^{-1})^{k_1 k_2} \ell_{k_1}(j, \hat{w}). \quad (124)$$

Therefore $\hat{w}_j - \hat{w} = O_p(1/n)$, resulting that $w^* - \hat{w} = O_p(1/n)$. It follows that

$$(\hat{w}_j)^{k_1} - \hat{w}^{k_1} = -\frac{1}{n} (L(\hat{w}, -j)^{-1})^{k_1 k_2} \ell_{k_2}(j, \hat{w}) + O_p(1/n^2)$$

$$= -\frac{1}{n} (L(\hat{w})^{-1})^{k_1 k_2} \ell_{k_2}(j, \hat{w}) + O_p(1/n^2), \quad (125)$$

where we used $L(w, -j) = L(w) + O_p(1/n)$. Hence

$$\frac{1}{n} \sum_{j=1}^{n} ((\hat{w}_j)^{k_1} - \hat{w}^{k_1})((\hat{w}_j)^{k_2} - \hat{w}^{k_2})$$

$$= \frac{1}{n^2} \sum_{j=1}^{n} (L(\hat{w})^{-1})^{k_1 k_3} \ell_{k_3}(j, \hat{w})(L(\hat{w})^{-1})^{k_2 k_4} \ell_{k_4}(j, \hat{w}) + O_p(1/n^3)$$

$$= \frac{1}{n^2} f_{k_1 k_3} f_{k_2 k_4} F_{k_3, k_4} + O_p(1/n^3), \quad (126)$$

which shows eq. (118) in Lemma 4. Let us show eq. (117). From eq. (120), by using the higher order mean value theorem, there exists a parameter $w^{**}$ which satisfies $\|w^{**} - \hat{w}\| \leq \|\hat{w}_j - \hat{w}\|$ and

$$\frac{1}{n} \ell_{k_1}(j, \hat{w}) + L_{k_1 k_2}(\hat{w}, -j)((\hat{w}_j)^{k_2} - \hat{w}^{k_2})$$

$$+ \frac{1}{2} L_{k_1 k_2 k_3}(w^{**}, -j)((\hat{w}_j)^{k_2} - \hat{w}^{k_2})(\hat{w}_j)^{k_3} - \hat{w}^{k_3}) = 0, \quad (127)$$

where we used eq. (123). The second term of eq. (127) is

$$L_{k_1 k_2}(\hat{w}, -j)((\hat{w}_j)^{k_2} - \hat{w}^{k_2})$$

$$= L_{k_1 k_2}(\hat{w})((\hat{w}_j)^{k_2} - \hat{w}^{k_2}) + \frac{1}{n} \ell_{k_1 k_2}(j, \hat{w})((\hat{w}_j)^{k_2} - \hat{w}^{k_2})$$

$$= L_{k_1 k_2}(\hat{w})((\hat{w}_j)^{k_2} - \hat{w}^{k_2}) - \frac{1}{n^2} \ell_{k_1 k_2}(j, \hat{w})(L(\hat{w})^{-1})^{k_2 k_3} \ell_{k_3}(j, \hat{w}) + O_p(1/n^3). \quad (128)$$

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where we used eq.\[(122)\] and eq.\[(125)\]. Also by eq.\[(125)\], the third term of eq.\[(127)\] is
\[
\frac{1}{2}L_{k_1k_2k_3}(w^{**}, -j)((\hat{w}_j)^{k_2} - \hat{w}^{k_2})(((\hat{w}_j)^{k_3} - \hat{w}^{k_3})
\]
\[
= \frac{1}{2}L_{k_1k_2k_3}(\hat{w})((\hat{w}_j)^{k_2} - \hat{w}^{k_2})(((\hat{w}_j)^{k_3} - \hat{w}^{k_3}) + O_p(\frac{1}{n^3})
\]
\[
= \frac{1}{2n^2}L_{k_1k_2k_3}(\hat{w})(L(\hat{w})^{-1})k_4k_5(j, \hat{w})(L(\hat{w})^{-1})k_5k_5(j, \hat{w}) + O_p(\frac{1}{n^3}). \tag{129}
\]
Then by applying eq.\[(128)\], eq.\[(129)\], \(L_{k_1}(\hat{w}) = 0\), and \((L^{-1})^{k_1k_2} = J^{k_1k_2}\) to eq.\[(127)\], the sum for \(j = 1, 2, ..., n\) of eq.\[(127)\] results in
\[
L_{k_1k_2}(\frac{1}{n} \sum_{j=1}^{n}((\hat{w}_j)^{k_2} - \hat{w}^{k_2})) - \frac{1}{n^2}F_{k_1k_2k_3}J^{k_2k_3}
\]
\[
+ \frac{1}{2n^2}L_{k_1k_2k_3}J^{k_2k_4}J^{k_3k_5}F_{k_4k_5} + O_p(\frac{1}{n^3}) = 0. \tag{130}
\]
Therefore
\[
\frac{1}{n} \sum_{j=1}^{n}((\hat{w}_j)^{k_1} - \hat{w}^{k_1}) = \frac{1}{n^2}J^{k_1k_2}J^{k_3k_4}F_{k_2k_3,k_4}
\]
\[
- \frac{1}{2n^2}J^{k_1k_2}J^{k_3k_4}J^{k_5k_6}L_{k_2k_3k_5}F_{k_4k_6} + O_p(\frac{1}{n^3}), \tag{131}
\]
which shows eq.\[(117)\] in Lemma 4. The last equation in Lemma 4, eq.\[(119)\], is proved by
\[
\frac{1}{n} \sum_{j=1}^{n}\{f(\hat{w}_j) - f(\hat{w})\} = \frac{1}{n} \sum_{j=1}^{n}((\hat{w}_j)^{k_1} - \hat{w}^{k_1})f_{k_1}
\]
\[
+ \frac{1}{2n} \sum_{j=1}^{n}((\hat{w}_j)^{k_1} - \hat{w}^{k_1})((\hat{w}_j)^{k_2} - \hat{w}^{k_2})f_{k_1k_2} + O_p(\frac{1}{n^3})
\]
\[
= \frac{1}{n^2}f_{k_1}(S^{k_1} - T^{k_1}/2) + \frac{1}{2n^2}f_{k_1k_2}U^{k_1k_2} + O_p(\frac{1}{n^3}), \tag{132}
\]
which completes Lemma 4. (Q.E.D.)

6 Proof of Theorem 1

In this section, we prove the main theorems. The proof of Theorem 1 consists of the five parts, Cross validation, WAIC, mathematical relations, averages, and random generalization loss.

6.1 Proof of Theorem 1, Cross Validation

In this subsection, we prove eq.\[(39)\] in Theorem 1. By Lemma 2,
\[
\mathbb{E}_{\phi_0}[\phi(w)] = \phi(\hat{w})(1 + \frac{R_1(\phi, \hat{w})}{\phi(\hat{w})n} + \frac{R_2(\phi, \hat{w})}{\phi(\hat{w})n^2}) + O_p(\frac{1}{n^3}), \tag{133}
\]
\[
\mathbb{E}_{\phi_0}^{(-j)}[\phi(w)] = \phi(\hat{w}_j)(1 + \frac{R_1(\phi, \hat{w}_j)}{\phi(\hat{w}_j)(n - 1)} + \frac{R_2(\phi, \hat{w}_j)}{\phi(\hat{w}_j)(n - 1)^2}) + O_p(\frac{1}{n^3}), \tag{134}
\]
For an arbitrary $C^\infty$-class function $f(w)$, by Lemma 4,
\[
\frac{f(\hat{w}_j)}{n-1} - \frac{f(\hat{w})}{n} = \frac{f(\hat{w}_j) - f(\hat{w})}{n-1} + \frac{f(\hat{w})}{n(n-1)} = \frac{f(\hat{w})}{n^2} + O_p\left(\frac{1}{n^3}\right),
\]
(135)
\[
\frac{f(\hat{w}_j)}{(n-1)^2} - \frac{f(\hat{w})}{n^2} = \frac{f(\hat{w}_j) - f(\hat{w})}{(n-1)^2} + \frac{(2n-1)f(\hat{w})}{n^2(n-1)^2} = O_p\left(\frac{1}{n^3}\right).
\]
(136)
By using Lemma 1 and by applying these equations for $f(w) = R_1(w)/\phi(w), R_2(w)/\phi(w)$,
\[
\text{CV}(\varphi) - \text{CV}(\varphi_0) = \frac{1}{n} \sum_{j=1}^{n} \{\log \mathbb{E}_{\varphi_0}[\varphi | \hat{w}_j] - \log \mathbb{E}_{\varphi_0}[\varphi | \hat{w}]\}
\]
\[
= \frac{1}{n} \sum_{j=1}^{n} \{\log \varphi(\hat{w}_j) - \log \varphi(\hat{w})\} + \frac{R_1(\hat{w})}{\varphi(\hat{w})n^2} + O_p\left(\frac{1}{n^3}\right).
\]
(137)
By using Lemma 2 and 4,
\[
\text{CV}(\varphi) - \text{CV}(\varphi_0) = \frac{1}{n^2}(\log \phi)_{k_1} (S_{k_1} - \frac{1}{2} T_{k_1}) + \frac{1}{2n^2}(\log \phi)_{k_1 k_2} U_{k_1 k_2}
\]
\[
+ \frac{1}{2n^2}(\phi_{k_1 k_2} J_{k_1 k_2} - \phi_{k_1} V_{k_1}) + O_p\left(\frac{1}{n^3}\right).
\]
(138)
Then by using
\[
\phi_{k_1} / \phi = (\log \phi)_{k_1},
\]
\[
\phi_{k_1 k_2} / \phi = (\log \phi)_{k_1 k_2} + (\log \phi)_{k_1} (\log \phi)_{k_2},
\]
it follows that
\[
\text{CV}(\varphi) - \text{CV}(\varphi_0) = \frac{1}{n^2}(\log \phi)_{k_1} (S_{k_1} - \frac{1}{2} T_{k_1} - \frac{1}{2} V_{k_1})
\]
\[
+ \frac{1}{2n^2}(\log \phi)_{k_1 k_2} (U_{k_1 k_2} + J_{k_1 k_2})
\]
\[
+ \frac{1}{2n^2}(\log \phi)_{k_1} (\log \phi)_{k_2} J_{k_1 k_2} + O_p\left(\frac{1}{n^3}\right),
\]
(139)
which completes eq.(39). (Q.E.D.)

6.2 Proof of Theorem 1, WAIC

In this subsection we prove eq.(41) and eq.(43) in Theorem 1. In the following, we prove eq.(43). In order to prove eq.(41), it is sufficient to prove eq.(43) in the case $\varphi(w)0 = \varphi_0(w)$ for an arbitrary $\varphi_0(w)$. Let the functional cumulant generating function for $\varphi_0(w)$ be
\[
F_{\text{cum}}^0(\alpha) = \frac{1}{n} \sum_{i=1}^{n} \log \mathbb{E}_{\varphi_0}[p(X_i | w)^\alpha].
\]
For a natural number $j$, we define the $j$th functional cumulant by

$$C_j(\alpha) \equiv \frac{\partial^j}{\partial \alpha^j} F_{\text{cum}}^0(\alpha).$$

Then by definition, $F_{\text{cum}}^0(0) = 0$ and

$$\begin{align*}
\text{CV}(\varphi_0) &= F_{\text{cum}}^0(-1), \\
\text{WAIC}(\varphi_0) &= T(\varphi_0) + V(\varphi_0)/n = -F_{\text{cum}}^0(1) + C_2(0).
\end{align*}$$

(140) (141)

For a natural number $j$, let $m_j(X_i, \alpha)$ be

$$m_j(X_i, \alpha) = \frac{\mathbb{E}_{\varphi_0}[\eta(X_i, w)^j \exp(-\alpha \eta(X_i, w))]}{\mathbb{E}_{\varphi_0}[\exp(-\alpha \eta(X_i, w))]},$$

where $\eta(X_i, w) = \log p(X_i|w) - \log p(X_i|\hat{w})$. Note that

$$\eta(X_i, w) = (w^{k_1} - \hat{w}^{k_1})\ell_{k_1}(X_i, \hat{w}) + O_P((w - \hat{w})^2).$$

(142)

Therefore, if $j$ is an odd number, by using Lemma 3,

$$m_j(X_i, \alpha) = O_P\left(\frac{1}{n^{(j+1)/2}}\right),$$

(143)

or if $j$ is an even number

$$m_j(X_i, \alpha) = O_P\left(\frac{1}{n^{j/2}}\right).$$

(144)

Since $p(X_i|\hat{w})$ is a constant function of $w$,

$$C_6(\alpha) = \frac{1}{n} \sum_{i=1}^n \frac{\partial^6}{\partial \alpha^6} \log \mathbb{E}_{\varphi_0}[p(X_i|w)^\alpha]$$

$$= \frac{1}{n} \sum_{i=1}^n \frac{\partial^6}{\partial \alpha^6} \log \mathbb{E}_{\varphi_0}[(p(X_i|w)/p(X_i|\hat{w}))^\alpha]$$

$$= \frac{1}{n} \sum_{i=1}^n \frac{\partial^6}{\partial \alpha^6} \log \mathbb{E}_{\varphi_0}[\exp(-\alpha \eta(X_i|w))]$$

$$= \frac{1}{n} \sum_{i=1}^n \left\{m_6 - 6m_5m_1 - 15m_4m_2 + 30m_4m_1^2 - 10m_3^2 + 120m_3m_2m_1 \right.$$  
$$- 120m_3m_1^3 + 30m_2^3 - 270m_2^2m_1^2 + 360m_2m_1^4 - 120m_1^6\} = O_p\left(\frac{1}{n^3}\right), \quad (145)$$

where $m_k = m_k(X_i, \alpha)$ in eq.(145). Hence by eq.(140),

$$\text{CV}(\varphi_0) = \sum_{j=1}^5 \frac{(-1)^j}{j!} C_j(0) + O_P\left(\frac{1}{n^3}\right). \quad (146)$$

On the other hand, by eq.(141),

$$\text{WAIC}(\varphi_0) = \sum_{j=1}^5 \frac{-1}{j!} C_j(0) + C_2(0) + O_P\left(\frac{1}{n^3}\right). \quad (147)$$
It follows that
\[
\text{WAIC}(\varphi_0) = CV(\varphi_0) - \frac{1}{12} C_4(0) + O_p(\frac{1}{n^3}).
\]
Hence the main difference between CV and WAIC is \(C_4(0)/12\). In order to prove eq.(43), it is sufficient to prove \(C_4(0) = O_p(1/n^3)\).

\[
C_4(0) = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial^4}{\partial \alpha^4} \log \mathbb{E}_\varphi [p(X_i|\alpha)]|_{\alpha=0}
\]
\[
= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial^4}{\partial \alpha^4} \log \mathbb{E}_\varphi [(p(X_i|w)/p(X_i|\hat{w}))^\alpha]|_{\alpha=0}
\]
\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ m_4 - 4m_3m_1 - 3m_2^2 + 12m_2m_1^2 - 6m_1^4 \right\}, \quad (148)
\]
where \(m_k = m_k(X_i, 0)\) in eq.(148). By eq.(143) and eq.(144),

\[
C_4(0) = \frac{1}{n} \sum_{i=1}^{n} \left\{ m_4(X_i, 0) - 3m_2(X_i, 0)^2 \right\} + O_p\left(\frac{1}{n^3}\right).
\]

By using a notation
\[
F_{k_1,k_2,k_3,k_4} \equiv \frac{1}{n} \sum_{i=1}^{n} \ell_{k_1}(X_i)\ell_{k_2}(X_i)\ell_{k_3}(X_i)\ell_{k_4}(X_i),
\]

it follows that by eq.(142) and Lemma 3,

\[
\frac{1}{n} \sum_{i=1}^{n} m_4(X_i) = \frac{3}{n^2} J_{k_1,k_2,k_3,k_4} F_{k_1,k_2,k_3,k_4} + O_p(1/n^3), \quad (149)
\]
\[
\frac{1}{n} \sum_{i=1}^{n} m_2(X_i)^2 = \frac{1}{n^2} J_{k_1,k_2,k_3,k_4} F_{k_1,k_2,k_3,k_4} + O_p(1/n^3), \quad (150)
\]
resulting that \(C_4(0) = O_p(1/n^3)\), which completes eq.(43). Then, eq.(41) is immediately derived using eq.(39) and eq.(43). (Q.E.D.)

6.3 Mathematical Relations between Priors

In this subsection, we prove eq.(44), eq.(45), and eq.(46). Since \(\hat{w}\) minimizes \(L(w)\),

\[
L_{k_1}(\hat{w}) = 0.
\]
There exists \(w^*\) such that \(\|w^* - w_0\| \leq \|\hat{w} - w_0\|\) and that

\[
L_{k_1}(w_0) + L_{k_1,k_2}(w_0)(\hat{w} - w_0) = 0.
\]
By the regularity condition (3), \(\hat{w} \to w_0\) resulting that \(w^* \to w_0\). By using the central limit theorem,

\[
\hat{w} - w_0 = (L_{k_1,k_2}(w^*))^{-1} L_{k_1}(w_0) = O_p\left(\frac{1}{\sqrt{n}}\right). \quad (151)
\]
Hence

\[ L_{k_1k_2}(w) = \mathbb{E}[L_{k_1k_2}(w)] + \frac{\beta_{k_1k_2}}{n^{1/2}}, \quad (152) \]
\[ L_{k_1k_2k_3}(w) = \mathbb{E}[L_{k_1k_2k_3}(w)] + \frac{\beta_{k_1k_2k_3}}{n^{1/2}}, \quad (153) \]
\[ F_{k_1k_2}(w) = \mathbb{E}[F_{k_1k_2}(w)] + \frac{\gamma_{k_1k_2}}{n^{1/2}}, \quad (154) \]
\[ F_{k_1k_2k_3}(w) = \mathbb{E}[F_{k_1k_2k_3}(w)] + \frac{\gamma_{k_1k_2k_3}}{n^{1/2}}, \quad (155) \]

where \( \beta_{k_1k_2}, \beta_{k_1k_2k_3}, \gamma_{k_1k_2} \) and \( \gamma_{k_1k_2k_3} \) are constant order random variables, whose expectation values are equal to zero. By the definitions,

\[ \mathcal{L}_{k_1k_2}(w) = \mathbb{E}[L_{k_1k_2}(w)] + O\left(\frac{1}{n}\right), \quad (156) \]
\[ \mathcal{L}_{k_1k_2k_3}(w) = \mathbb{E}[L_{k_1k_2k_3}(w)] + O\left(\frac{1}{n}\right), \quad (157) \]
\[ \mathcal{F}_{k_1k_2}(w) = \mathbb{E}[F_{k_1k_2}(w)] + O\left(\frac{1}{n}\right), \quad (158) \]
\[ \mathcal{F}_{k_1k_2k_3}(w) = \mathbb{E}[F_{k_1k_2k_3}(w)] + O\left(\frac{1}{n}\right), \quad (159) \]

Let \( \beta \equiv \{\beta_{k_1k_2}\} \) and \( \Lambda \equiv \{L_{k_1k_2}(w)\} \). Then by eq. (152) and eq. (156),

\[
\mathcal{J}(w) = \mathbb{E}[\Lambda]^{-1} + O\left(\frac{1}{n}\right) \\
= (\Lambda - \beta/\sqrt{n})^{-1} + O\left(\frac{1}{n}\right) \\
= (\Lambda(1 - \Lambda^{-1} \beta/\sqrt{n}))^{-1} + O\left(\frac{1}{n}\right) \\
= (1 + \Lambda^{-1} \beta/\sqrt{n})^{-1} + O\left(\frac{1}{n}\right) \\
= J(w) + \Lambda^{-1} \beta \Lambda^{-1}/\sqrt{n} + O\left(\frac{1}{n}\right).
\]

Hence

\[
J^{k_1k_2}(w) = \mathcal{J}^{k_1k_2}(w) + O_p(1/\sqrt{n}), \\
\mathbb{E}[J^{k_1k_2}(w)] = \mathcal{J}^{k_1k_2}(w) + O(1/n).
\]

It follows that

\[
M(\phi, w_0) = \mathcal{M}(\phi, w_0) + O_p(1/\sqrt{n}), \\
\mathbb{E}[M(\phi, w_0)] = \mathcal{M}(\phi, w_0) + O(1/n).
\]

Hence

\[
M(\phi, \hat{w}) = M(\phi, w_0) + (\hat{w} - w_0)^{k_1}(M(\phi, w_0))_{k_1} = M(\phi, w_0) + O_p\left(\frac{1}{\sqrt{n}}\right), \\
\mathbb{E}[M(\phi, \hat{w})] = M(\phi, w_0) + O\left(\frac{1}{n}\right),
\]

which shows eq. (44) and eq. (45). Then eq. (45) is immediately derived by the fact \( \hat{w} - \mathbb{E}_\phi[w] = O_p(1/n) \) by Lemma 3. (Q.E.D.)

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6.4 Proof of Theorem 1, Averages

In this subsection, we prove we show eq.(40), eq.(42), and eq.(48).

Firstly, eq.(40) is derived from eq.(39) and eq.(46). Secondly, eq.(42) is derived from eq.(41) and eq.(46). Lastly, let us prove eq.(48). Let $CV_n(\varphi)$ and $G_n(\varphi)$ be the cross validation and the generalization losses for $X^n$, respectively. Then by the definition, for an arbitrary $\varphi$,

$$
E[G_n(\varphi)] = E[CV_{n+1}(\varphi)] \\
= E[CV_{n+1}(\varphi_0)] + \frac{E[M(\varphi, \hat{w})]}{(n+1)^2} + O\left(\frac{1}{n^3}\right)
$$

Since $\bar{\varphi}$ minimizes $w$, we used $1/n^2 - 1/(n+1)^2 = O(1/n^3)$, which completes eq.(48). (Q.E.D.)

6.5 Proof of Theorem 1, Random Generalization Loss

In this subsection, we prove eq.(47) in Theorem 1. We use a notation $\ell(n + 1, w) = \log p(X_{n+1}|w)$. Let $\hat{w}$ be the parameter that minimizes

$$
-\frac{1}{n+1} \sum_{i=1}^{n+1} \log p(X_i|w) - \frac{1}{n+1} \log \varphi(w) = \frac{n}{n+1} \left\{ \ell(w) - \frac{1}{n} \ell(n+1, w) \right\}.
$$

Since $\hat{w}$ minimizes $L(w) - \ell(n+1, w)/n$,

$$
L_{k_1}(\hat{w}) - \frac{1}{n} \ell_{k_1}(n+1, \hat{w}) = 0. \quad (161)
$$

By applying the mean value theorem to eq.(161), there exists $\bar{w}^*$ such that

$$
L_{k_1}(\hat{w}) + (\bar{w}^{k_2} - \hat{w}^{k_2}) L_{k_1k_2}(\bar{w}^*) - \frac{1}{n} \ell_{k_1}(n+1, \bar{w}) = 0.
$$

By using $L_{k_1}(\hat{w}) = 0$ and positive definiteness of $L_{k_1k_2}(\bar{w})$,

$$
\bar{w}^{k_2} - \hat{w}^{k_2} = O_p\left(\frac{1}{n}\right). \quad (162)
$$

By applying the higher order mean value theorem to eq.(161), there exists $w^{**}$ such that

$$
(\bar{w}^{k_2} - \hat{w}^{k_2}) L_{k_1k_2}(\bar{w}) + \frac{1}{2} (\bar{w}^{k_2} - \hat{w}^{k_2}) (\bar{w}^{k_3} - \hat{w}^{k_3}) L_{k_1k_2k_3}(\bar{w}^{**}) - \frac{1}{n} \ell_{k_1}(n+1, \bar{w}) = 0.
$$

By eq.(162), the second term of this equation is $O_p(1/n^2)$. The inverse matrix of $L_{k_1k_2}(\hat{w})$ is $J_{k_1k_2}(\hat{w})$,

$$
\bar{w}^{k_1} - \hat{w}^{k_1} = \frac{1}{n} J_{k_1k_2}(\hat{w}) \ell_{k_2}(n+1, \hat{w}) + O_p\left(\frac{1}{n^2}\right). \quad (163)
$$

By eq.(161), $\hat{w} - w_0 = O_p(1/\sqrt{n})$. Hence by the expansion of $(\hat{w} - w_0)$,

$$
E_{X_{n+1}}[\ell_{k_2}(n+1, \hat{w})] = E_{X_{n+1}}[(\log p(X_{n+1} | \hat{w}))_{k_2}] \\
= (\bar{w}^{k_3} - (w_0)^{k_3}) E_{X_{n+1}}[(\log p(X_{n+1} | w_0))_{k_2}] + O_p\left(\frac{1}{n}\right), \quad (164)
$$
where we used \( \mathbb{E}_{X_{n+1}}[(\log p(X_{n+1}|w_0))_{k_2}] = 0 \). By eq. (103) and eq. (104),

\[
\mathbb{E}_{X_{n+1}}[\tilde{w}^{k_1} - w^{k_1}] = -\frac{1}{n}J^{k_1k_2}(\tilde{w})(\tilde{w}^{k_3} - (w_0)^{k_3})\mathbb{E}[L_{k_2k_3}(w_0)] + O_p(\frac{1}{n^2})
\]

\[
= -\frac{1}{n}(\tilde{w}^{k_1} - (w_0)^{k_1}) + O_p(\frac{1}{n^2}),
\]

where we used \( J^{k_2k_3}(\tilde{w}) = (\mathbb{E}[L_{k_2k_3}(w_0)])^{-1} + O_p(1/n^{1/2}) \). Therefore, by Lemma 1 and 2

\[
G(\varphi) - G(\varphi_0) = -\mathbb{E}_{X_{n+1}}[\log \mathbb{E}[\varphi^{*(n+1)}][\varphi(w)] - \log \mathbb{E}[\varphi(w)]]
\]

\[
= -\mathbb{E}_{X_{n+1}}[-\log(\phi(\tilde{w}) + \frac{R_1(\phi, \tilde{w})}{n + 1}) + \log(\phi(\tilde{w}) + \frac{R_1(\phi, \tilde{w})}{n})] + O_p(\frac{1}{n^2})
\]

\[
= -\mathbb{E}_{X_{n+1}}[(\tilde{w}^{k_1} - w^{k_1})(\log \phi)_{k_1}(\tilde{w}) + O_p(\frac{1}{n^2})]
\]

\[
= \frac{1}{n}(\tilde{w}^{k_1} - (w_0)^{k_1})(\log \phi)_{k_1}(\tilde{w}) + O_p(\frac{1}{n^2}).
\]

(165)

By eq. (151), \( \hat{w} - w_0 = O_p(1/\sqrt{n}) \), we obtain eq. (47). (Q.E.D.)

### 6.6 Proof of Theorem 2

If there exists a parameter which satisfies \( q(x) = p(x|w_0) \), then \( \tilde{w} - w_0 = O_p(1/\sqrt{n}) \), \( \langle L_{k_1k_2}(w) = L_{k_1k_2}(w) + O_p(1/\sqrt{n}) \), \( \langle L_{k_1k_2k_3}(w) = L_{k_1k_2}(w) + O_p(1/\sqrt{n}) \), \( \langle F_{k_1k_2}(w) = F_{k_1k_2}(w) + O_p(1/\sqrt{n}) \), and \( \langle F_{k_1k_2k_3}(w) = F_{k_1k_2k_3}(w) + O_p(1/\sqrt{n}) \). Hence Theorem 2 is obtained. (Q.E.D.)

### 7 Discussions

In this chapter, we discuss several points about predictive prior design.

#### 7.1 Summary of Results

In this paper, we have shown the mathematical properties of Bayesian CV, WAIC, and the generalization loss. Let us summarize the results of this paper.

1. Even if the posterior distribution is not normal or even if the true distribution is unrealizable by a statistical model, CV and WAIC are applicable to predictive prior design. Theoretically CV and WAIC are asymptotically equivalent, whereas experimentally the variance of WAIC is a little smaller than CV. In the regularity conditions are satisfied, then CV and WAIC can be approximated by WAICR. The variance of WAICR is a little smaller than CV and WAIC.

2. If the true distribution is realizable by a statistical model, then CV and WAIC can be estimated by WAICRS. The variance of WAICRS is very smaller than WAICR.

3. If the posterior distribution is rigorously normal and if the true distribution is realizable by a statistical model, then DIC is almost equal to WAICRS. If otherwise, then DIC is different from CV, WAIC, or WAICRS and the chosen hyperparameter by DIC is not optimal for predictive prior design in general.

4. The marginal likelihood is not appropriate for predictive prior design.
7.2 Divergence Phenomenon of CV and WAIC

In this subsection we study a divergence phenomenon of CV, WAIC, and the marginal likelihood. Let the maximum likelihood estimator be $w_{\text{mle}}$ and $\delta_{\text{mle}}(w) = \delta(w - w_{\text{mle}})$. Then for an arbitrary proper prior $\varphi(w)$, $\text{CV}(\varphi) \geq \text{CV}(\delta_{\text{mle}})$, $\text{WAIC}(\varphi) \geq \text{WAIC}(\delta_{\text{mle}})$, and $F_{\text{free}}(\varphi) \geq F_{\text{free}}(\delta_{\text{mle}})$. Hence, if a candidate prior can be made to converge to $\delta_{\text{mle}}(w)$, then minimizing these criteria results in the maximum likelihood method, where Theorem 1 does not hold.

Assume that a proper prior $\varphi(w) = \varphi(w|\lambda)$ has a hyperparameter $\lambda$. The set of divergent parameters of $\varphi(w|\lambda)$ is defined by

$$W_{\text{div}}(\varphi) = \{w \in W; \text{ There exists } \{\lambda_k\} \text{ s.t. } \lim_{k \to \infty} \varphi(w|\lambda_k) \to \delta(w - \overline{w})\}.$$

For example, if $\varphi(w|\lambda) = \sqrt{\lambda}/2\pi \exp(-\lambda w^2/2)$, then $W_{\text{div}}(\varphi) = \{0\}$, because $\lambda_k = k$ gives a sequence of priors which converges to the delta function.

If the optimal parameter $w_0$ that minimizes the average generalization loss is contained in $W_{\text{div}}(\varphi)$, then the optimal hyperparameter does not remain in a compact set as $n \to \infty$. For example, the optimal hyperparameter for WAICRS in eq.(80) diverges if $\hat{w} \to 0$. In such cases, CV or WAIC may not have any minimum point, then the hyperparameter cannot be optimized by using CV or WAIC. In such cases, some hyperprior or regularization term which is necessary. It is an important study to clarify the set of divergent parameters of a given prior. For example, if the Dirichlet distribution on $a \in (0,1)$

$$\text{Dir}(a|\lambda_1, \lambda_2) = C(\lambda_1, \lambda_2)a^{\lambda_1}(1-a)^{\lambda_2},$$

is used as a prior, then an arbitrary parameter in $(0,1)$ is contained in $W_{\text{div}}(\text{Dir})$, because

$$\text{Dir}(a|b_0k, c_0k) \to \delta(a - b_0/(b_0 + c_0)) \ (k \to \infty).$$

7.3 Training and Testing Sets

In practical applications of machine learning, we often prepare both a set of training samples $X^n$ and a set of test samples $Y^m$, where $X^n$ and $Y^m$ are independent. This method is sometimes called the holdout cross validation. Then we have a basic question, “Does the optimal hyperparameter chosen by CV or WAIC using a training set $X^n$ minimize the generalization loss estimated using a test set $Y^n$ ?” The theoretical answer to this question is No, because, as is shown in Theorem 1, the optimal hyperparameter for $X^n$ asymptotically minimizes $\mathbb{E}[G(X^n)]$ but not $G(X^n)$. If one would find the hyperparameter which minimizes $G(X^n)$, then neither CV, WAIC, DIC, nor the marginal likelihood is appropriate. On the other hand, if one wants to measure the optimality of the chosen hyperparameter by the criterion $\mathbb{E}[G(X^n)]$, then CV or WAIC using $Y^m$ is useful, because the optimal hyperparameter using $X^n$ is asymptotically equal to that using $Y^m$.

7.4 Self-Averaging and Bootstrap

In this paper, we have shown that the optimal hyperparameter for the minimum average generalization loss can be found by CV and WAIC asymptotically. However, the variance of the estimated hyperparameter is sometimes not small. In experiments, WAICRS has very smaller variances than CV and WAIC. Although WAICRS can be used only in the
case when the true distribution is realizable by a statistical model, it may be useful by its small variance.

If a statistical model $p(x|w)$ is complicated and if it is difficult to derive the mathematical form of WAICRS, then it can be estimated numerically by

$$\text{WAICRS} \approx E_{Y^n}[\text{WAIC}(Y^n, \varphi) - \text{WAIC}(Y^n, \varphi_0)]$$

where $Y^n$ is taken from the Bayesian predictive distribution $p^*(x)$ and WAIC($Y^n, \varphi$) is WAIC for a set $Y^n$. Moreover, if $Y^n$ is taken from the empirical distribution $(1/n) \sum \delta(x - X_i)$, then the above equation approximates WAICR. These numerical methods may need heavy computational costs, however, they may be useful if the precise hyperparameter optimization is necessary.

8 Conclusion

In this paper, we studied several methods how to design the hyperparameter from the predictive point of view. The mathematical relation between priors gives the explicit criterion of the prior and its variance is made smaller by using self-averaging. To construct the generalized theory of this paper onto singular statistical model is the important problem for future study.

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