Approximate cross–validation formula for Bayesian linear regression*

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Abstract— Cross–validation (CV) is a technique for evaluating the ability of statistical models/learning systems based on a given data set. Despite its wide applicability, the rather heavy computational cost can prevent its use as the system size grows. To resolve this difficulty in the case of Bayesian linear regression, we develop a formula for evaluating the leave-one-out CV error approximately without actually performing CV. The usefulness of the developed formula is tested by statistical mechanical analysis for a synthetic model. This is confirmed by application to a real-world supernova data set as well.

I. INTRODUCTION

Consider carrying out linear regression analysis for a data set $D^M = \{(x_\mu, y_\mu)\}_{\mu=1}^M$, where $x_\mu = (x_i) \in \mathbb{R}^N$ and $y_\mu \in \mathbb{R}$. The linear regression model assumes that the relationship between $y_\mu$ and $x_\mu$ is linear, which indicates that the model takes the form

$$y_\mu = x_\mu^T w + n_\mu, \quad \mu = 1, 2, \ldots, M$$

(1)

using the parameter vector $w = (w_i) \in \mathbb{R}^N$. Here, $\mathbb{T}$ represents the matrix-vector transpose operation, $n_\mu$ indicates noise and the intercept term is omitted for simplicity. The parameter vector $w$ can be determined uniquely by the least square method if $M \geq N$. However, in some contexts such as compressed sensing and certain kinds of high-dimensional data analysis, one needs to infer $w$ even when $M < N$. The Bayesian framework offers a useful strategy for coping with such demands. For this, we introduce a sparse prior probability distribution $P(w|\rho) = \prod_{i=1}^N \phi(w_i|\rho)$, where $\phi(w_i|\rho) = (1 - \rho)\delta(w_i) + \rho f(w_i)$, $0 \leq \rho \leq 1$ and $f(w)$ is a density function that does not have finite mass at $w = 0$, which effectively suppresses the $w$ degree of freedom. This formally yields the posterior distribution

$$P(w|D^M; \beta, \rho) = \frac{e^{\beta \text{RSS}(w|D^M)} \prod_{i=1}^N \phi(w_i|\rho)}{Z(D^M; \beta, \rho)},$$

(2)

where $\beta^{-1}$ corresponds to the variance of noise,

$$Z(D^M; \beta, \rho) = \int e^{\beta \text{RSS}(w|D^M)} \prod_{i=1}^N \phi(w_i|\rho) dw,$$

(3)

and

$$\text{RSS}(w|D^M) = \frac{1}{2} \sum_{\mu=1}^M (y_\mu - x_\mu^T w)^2$$

(4)

means the residual sum of squares (RSS). Based on (2), one can set the posterior mean

$$\langle w \rangle = \int w P(w|D^M; \beta, \rho) dw$$

(5)

as a reasonable estimator of the parameter vector $w$ since it considerably reduces (4) when the hyper-parameters $\beta$ and $\rho$ are appropriately tuned.

However, there are two obstacles to making this procedure practical. The first one is the computational difficulty of evaluating (5). For this, one of the current authors has developed an approximation method [1], which can be utilized for systems of reasonable sizes. The other issue, which we would like to address here, is how to determine $\beta$ and $\rho$. If $D^M$ is actually generated by the process of (1) using a true parameter vector $w^0$ that follows the sparse prior $P(w|\rho)$ and Gaussian noises, then maximization of the marginal likelihood $P(D^M; \beta, \rho) = \int P(D^M|w, \beta) P(w|\rho) dw = Z(D^M; \beta, \rho)/(2\pi\beta^{-1})^{M/2}$ would be the most rational approach. Unfortunately, in practice, there are many situations where we cannot expect these assumptions to hold. In such cases, especially when the objective of the regression is to maximize the prediction ability for novel samples, minimizing the cross–validation (CV) error is a dominant alternative.

CV is a general framework for evaluating the prediction ability of statistical models/learning systems based on a given data set. Despite its wide applicability, the heavy computation cost can make it difficult to use. The purpose of this paper is to show that, in the case of the Bayesian linear regression, employment of the approximation method of [1] naturally enables us to evaluate, approximately, the leave-one-out (LOO) CV error without actually performing CV, which considerably reduces the computational cost. The usefulness will also be tested by applications to a synthetic problem and a real world data analysis.

II. RELATED WORK

There have been several studies of CV for linear regression. The analytical formula for evaluating the LOO CV error (LOOE) exactly, without actually performing CV, is widely known for standard linear regression and ridge regression [2]. This formula was extended to the case in which linear constraints are present [3]. An alternative measure, which has a property similar to that of LOOE and can be evaluated at a lower computational cost, was proposed as the “generalized...
cross-validation” in [4] for regularized linear regression. Two types of LOOE approximation formulas for LASSO were recently provided in [5]. In contrast to these, our aim here is to develop a computationally feasible approximate formula to evaluate LOOE in the Bayesian formalism in which sparse (singular) priors can be employed. A similar attempt has been made for feedforward neural networks in [6].

III. CROSS-VALIDATION IN BAYESIAN LINEAR REGRESSION

A. Expectation consistent (EC) approximation

As the basis of our study, we briefly mention the approximate inference scheme for Bayesian linear regression developed in [1] and summarized in the following two theorems.

Theorem 1: Let us define Gibbs free energy as
\[
\Phi(m|D; \beta, \rho) = \text{extr}_h \left\{ h \cdot m - \ln \left( \int e^{-\beta \text{RSS}(u|D; m)} \prod_{i=1}^{N} \phi(u_i|m) e^{h \cdot w} dw \right) \right\}
\]
where \(\text{extr}_u \{ f(u) \}\) generally means the extremization of a function \(f(u)\) with respect to \(u\). The function \(\Phi(m|D; \beta, \rho)\) is a downward-convex function of \(m = (m_i) \in \mathbb{R}^N\) and its unique minimizer accords to (5).

Theorem 2: To characterize the property of the \(N \times M\) data matrix \(X = (x_{ij})\), we introduce the function
\[
G(x) = \text{extr}_w \left\{ -\frac{1}{2N} \ln \det (\Lambda - XX^T) - \frac{\Lambda x}{2} \right\}
\]
The expectation consistent (EC) approximation [7], requiring matching of the first and the macroscopic second moments, approximately evaluates (5) as
\[
\Phi(m|D; \beta, \rho) \simeq \Phi_{\text{EC}}(m|D; \beta, \rho)
= \text{extr}_{Q,E,h} \left\{ \beta \text{RSS}(m|D) - NQ - (\beta(Q - q)) - \frac{N \text{EQ}}{2} \right. \\
+ h \cdot m - \sum_{i=1}^{N} \ln \left[ \phi(u_i|m) e^{-\frac{1}{2} w^2 + h \cdot w} dw_i \right] \\
+ \text{const}
\]
for large systems, where \(q = N^{-1}|m|^2\).

The detailed derivations of the two theorems are provided in [1]. These theorems indicate that the Bayesian estimator of the parameter vector can be evaluated approximately by minimizing the EC free energy (8). Unfortunately, the minimization is non-trivial to perform, and various methods have been proposed for accomplishing this task [8]–[10]. However, when the dimensionality \(N\) is “moderately large,” Newton’s method works pretty well, and we here regard it as a default solver. More concretely, one can obtain a solution of the EC approximation as a convergent point of the following discrete dynamics counted by \(t = 1, 2, \ldots\):
\[
m^{t+1} = m^t - (\partial_m^2 \Phi_{\text{EC}})^{-1} \partial_m \Phi_{\text{EC}},
\]
where
\[
\partial_m \Phi_{\text{EC}} = -\beta X (y - X^T m^t) - E^t m^t + h^t,
\]
and
\[
\partial_m^2 \Phi_{\text{EC}} = \beta XX^T + \left( \frac{1}{M_t^2 - (m_t^i)^2} - E^t \right) \delta_{ij},
\]
and \(y = (y_i)\). Here, \(h^t = (h^t_i)\) and \(E^t\) stand for the extremized values of \(h = (h_i)\) and \(E\) for \(m = (m_t^i)\) at the right hand side of (8), respectively, and \(M_t = -2(\partial \eta / \partial E^t) \ln \left[ \int \phi(u_i|m) e^{-\frac{1}{2} w^2 + h^t_i w} dw_i \right]\). For simplicity, terms of \(O(N^{-1})\) are omitted in (11).

The most time-consuming part in the above calculation is the matrix inversion operation required in (11). Therefore, the computation cost per update scales roughly as \(O(N^3)\).

B. Cross-validation (CV)

The EC approximation offers an approximate estimate of (5) for a given pair of hyper-parameters \(\beta\) and \(\rho\). However, in many situations, their correct values are not provided in advance and have to be determined from \(D^M\). The minimized value of (5) generally corresponds to the negative logarithm of the partition function \(Z(D^M; \beta, \rho)\). As \(Z(D^M; \beta, \rho)\) is proportional to the marginal likelihood function \(P(D^M; \beta, \rho)\), determining \(\beta\) and \(\rho\) such that they minimize \(\min_m \{ \Phi_{\text{EC}}(m|D^M; \beta, \rho) \}\) is a reasonable strategy in terms of the maximum likelihood principle. Indeed, Ref. [11] reports that a similar strategy exhibits an excellent inference performance for signal recovery of compressed sensing. Nevertheless, this is not necessarily the case when the correct posterior cannot be expressed by the assumed model class, which would be more common in practice.

In such cases, under the assumption that the data \((x_{\mu}, y_{\mu})\) of \(\mu = 1, 2, \ldots, M\) are generated independently from an identical distribution, maximizing the prediction ability for novel samples, is an alternative guideline for determining the hyper-parameters. When no extra data is available other than \(D^M\), CV is a widely used method for estimating the prediction ability, which measures the prediction ability, is computed as the average RSS for the prediction over the test subsets. This means that performing the CV procedure many times for optimizing \(\beta\) and \(\rho\). Although the minimization of (5) for the \(k\) choices of test subsets is easily parallelized, the heavy computational cost could make the CV-based hyperparameter determination practically infeasible.

C. Leave-one-out (LOO) CV and its approximate formula

To reduce the computational cost, let us develop an approximate formula that estimates the CV error without performing CV. For this, we take particular note of LOO CV, which corresponds to \(k = M\). As the size of each test
subset of LOO CV is only unity, the differences between the estimators of an LOO and the full data sets is expected to be small. This enables us to evaluate the estimator of the LOO data set from that of the full data set in a perturbative manner, which yields a semi-analytic formula to evaluate the CV error based on the result of the EC approximation for the full data set $D^M$.

The fixed–point condition of (9), which can be read as

$$m_i = f(h_i; E),$$

$$h_i = \beta \sum_{\mu=1}^{M} x_{i\mu}(y_{\mu} - \sum_{j=1}^{N} x_{j\mu} m_j) + E m_i,$$ (12)

constitutes the basis for implementing the above idea. Here, we have defined a function $f(h; E)$ by

$$f(h; E) = \frac{\partial}{\partial h} \ln \left[ \int \phi(w|\rho)e^{-\frac{1}{2}w^2 + hw} dw \right].$$

Let us denote the solution of (12) and (13) for the “$\mu$-th LOO system,” which is defined by leaving the $\mu$-th data $(x_{\mu}, y_{\mu})$ out from the full data set, as $m_{i\rightarrow\mu}$ and $h_{i\rightarrow\mu}$. Since the contribution of the $\mu$-th data $(x_{\mu}, y_{\mu})$ to (12) and (13) is supposed to be small, the relation

$$h_{i\rightarrow\mu} \simeq h_{i\rightarrow\mu} + \Delta h_{i\rightarrow\mu}$$

is regarded as small. This indicates that the relation

$$m_i \simeq m_{i\rightarrow\mu} + \sum_{j=1}^{N} c_{ij}^\mu \Delta h_{j\rightarrow\mu},$$ (15)

holds between $m_i$ and $m_{i\rightarrow\mu}$, where $c_{ij}^\mu$ represents the rate of change of $m_{i\rightarrow\mu}$ when $h_{j\rightarrow\mu}$ is slightly changed.

To evaluate $c_{ij}^\mu$, we add the “external fields” $\theta_j$ to $h_{j\rightarrow\mu}$ for $\forall j \in \{1, 2, \ldots, N\}$ in (12) of the $\mu$-th LOO system, and take the partial derivative with respect to $\theta_j$ for $\forall j$ at $\theta_j = 0$ [7]. This yields a set of $N^2$ coupled equations

$$c_{ij}^\mu = (M_i - m_i^2) \left( \delta_{ij} - \beta \sum_{k=1}^{N} x_{i\nu} x_{j\nu} c_{k\nu}^\mu + E c_{ij}^\mu \right),$$ (16)

where we used the relation $\partial f(h_{i\rightarrow\mu}; E)/\partial h_{i\rightarrow\mu} = M_{i\rightarrow\mu} - m_{i\rightarrow\mu}^2 \simeq M_i - m_i^2$. The solution of (16) is given as

$$(c_{ij}^\mu) = (\partial^2 \Phi_{EC} - \beta x_{\mu} x_{\mu}^\top)^{-1}$$ (17)

in the matrix expression, where $\partial^2 \Phi_{EC}$ stands for the Hessian of the EC free energy (8) at the full estimator $m = (m_i)$.

The expressions (15) and (17) can be employed to evaluate the CV error of the $\mu$-th LOO estimator $(m_{i\rightarrow\mu})$ on the $\mu$-th data $(x_{\mu}, y_{\mu})$ using the full estimator $m = (m_i)$. For this, we evaluate the residual of the $\mu$-th LOO estimator on $(x_{\mu}, y_{\mu})$ utilizing (14) and (15) as

$$y_{\mu} - \sum_{i=1}^{N} x_{i\mu} m_{i\rightarrow\mu} \simeq y_{\mu} - \sum_{i=1}^{N} x_{i\mu} m_i$$

$$= \left(1 + \beta \sum_{i,j} x_{i\mu} x_{j\mu} c_{ij}^\mu \right) \left(y_{\mu} - \sum_{i=1}^{N} x_{i\mu} m_i\right)$$

$$= \left(1 - \beta x_{\mu}^\top (\partial^2 \Phi_{EC})^{-1} x_{\mu} \right) \left(y_{\mu} - \sum_{i=1}^{N} x_{i\mu} m_i\right),$$ (18)

where we used the Sherman-Morrison formula for the matrix inversion to simplify the expression. This means that LOE can be evaluated approximately as

$$\epsilon_{LOE} \equiv \frac{1}{2M} \sum_{\mu=1}^{M} \left( y_{\mu} - \sum_{i=1}^{N} x_{i\mu} m_{i\rightarrow\mu} \right)^2$$

$$\simeq \frac{1}{2M} \sum_{\mu=1}^{M} \left( 1 - \beta x_{\mu}^\top (\partial^2 \Phi_{EC})^{-1} x_{\mu} \right)^2.$$ (19)

To evaluate LOE literally, we need to solve the minimization problem of (8) for $M$ LOO systems, which requires $O(M N^3)$ computational costs, even if the necessary number of iterations for convergence of (9) is $O(1)$. On the other hand, the approximate LOE formula of (19) is expressed by using the solution of the full system only. In (9), we need to evaluate the matrix inversion of the Hessian $\partial^2 \Phi_{EC}$, which requires $O(N^3)$ computations. However, this is already computed when performing (9) to obtain the full solution, and does not require any extra computation cost. This means that the approximate formula accelerates the computation of LOE by a factor $M$.

IV. NUMERICAL VALIDATION

A. Synthetic model

We first examine the usefulness of the developed CV formula by applying it to a synthetic model in which the vector $y$ is generated in the manner of (1) on the basis of a true sparse vector $w^0 = (w_i^0)$. For analytical tractability, we assume that $X$ is a simple random matrix whose entries are sampled independently from $N(0, N^{-1})$, and that $w_i^0 (i = 1, 2, \ldots, N)$ and $n_i$ ($i = 1, 2, \ldots, M$) are also independently generated from $\phi(w|\rho_0, \sigma^2_0) = (1 - \rho_0)\delta(w) + \rho_0 N(0, \sigma^2_0)$ and $N(0, \sigma^2_0)$, respectively. Under these assumptions, the replica method of statistical mechanics makes it possible to assess theoretically the typical values of various macroscopic quantities as $N, M \to \infty$ while keeping $\alpha = M/N$ finite [1], [12]. We performed the theoretical assessment under the so-called replica symmetric assumption.

In the experiment, the system size was set to $N = 1000$, and the system parameters were fixed to $\rho_0 = 0.1$, $\alpha = 0.5$, $\sigma^2_0 = 10$, and $\sigma^2_0 = 0.1$. We estimated $w^0$ following the Bayesian linear regression utilizing the EC approximation [9]. The prediction ability of the Bayesian estimator is optimized when the correct sparse prior $\phi(w|\rho_0, \sigma^2_0)$ and
Fig. 1. Comparison between theory and experiment for $K$ by
$\sqrt{\text{error bars}}$ which represent the standard deviations among those samples divided.
Experimental samples exhibit good consistency with the theoretical estimates of
(red crosses) and LOOE assessed by the approximate formula
changing hyper-parameters
$a_i$.

| $K$ | 1    | 2    | 3    | 4    | 5    | 6    |
|-----|------|------|------|------|------|------|
| Approx. | 0.0328 | 0.0235 | 0.0219 | 0.0218 | 0.0220 | 0.0222 |
| Literal | 0.0327 | 0.0231 | 0.0220 | 0.0218 | 0.0218 | 0.0219 |
| RSS   | 0.0312 | 0.0178 | 0.0163 | 0.0156 | 0.0152 | 0.0150 |

TABLE I
LOOE S OBTAINED FOR $K = 1–6$ FOR TYPE Ia SUPERNOVA DATA SET.

$\beta = \sigma_{w_0}^2$ are employed. However, such information is not
available in many practical situations. To examine whether
the approximate CV formula [19] offers a clue to optimize
the prediction ability or not, we set the prior as $\phi(w|\rho, \sigma^2_w)$
and evaluated [19] changing hyper-parameters $\beta$, $\rho$, and $\sigma^2_w$.

Figure 1 shows the result obtained by varying $\beta$ while
setting the remaining two hyper-parameters to the correct
values $\rho = \rho_0$ and $\sigma^2_w = \sigma_{w_0}^2$. The curves represent the
theoretical estimate of the typical value of achieved RSS
per data $\epsilon = (1/2M) \sum_{i=1}^{M} (y_i - x_i^T \mu)^2$ (red curve) and
that of the prediction error for a new (1-st) data $\epsilon_\rho =
(1/2)(y_{i+1} - x_{i+1}^T \mu)^2$ (blue curve). Although $\epsilon$ decreases
monotonically as $\beta$ grows, which indicates overfitting to the
given data $D^M$, $\epsilon_\rho$ is minimized at the correct value $\beta = \sigma_{n0}^{-2} = 10$.
The symbols stand for experimentally evaluated $\epsilon$
(red crosses) and LOOE assessed by the approximate formula
[19] $\epsilon_{\text{LOO}}$ (blue circles), which were obtained from 30 experi-
mental samples. These samples exhibit good consistency
with the theoretical estimates of $\epsilon$ and $\epsilon_\rho$. Especially,
the consistency between $\epsilon_\rho$ and $\epsilon_{\text{LOO}}$ means that [19] offers a
reliable estimate of the prediction error based on a given
data set. This would be useful for determining the hyper-
parameters to optimize the prediction ability. Similar results
are obtained when $\rho$ and $\sigma^2_w$ are varied.

B. Type Ia Supernova data set

We also applied our methodology to a data set from
the SuperNova DataBase (SNDB) provided by the Berkeley
SuperNova Ia program [13], [14]. Screening based on a
certain criteria yields a reduced data set of $M = 78$
and $N = 276$ [15]. The purpose of the data analysis is
to construct a formula to estimate accurately the absolute
magnitude at the maximum of type Ia supernovae by linear
regression. To estimate this quantity accurately is particularly
important in modern astronomy because it directly influences
the measurement of long distances in the universe.

Following the conventional treatment of linear regression,
we preprocessed both the absolute magnitude at the
maximum (dependent variable) and the 276 candidates of
explanatory variables, which are composed of processed
spectral data, to have zero means. We applied the EC
approximation of the Bayesian sparse linear regression to the
preprocessed data set. As the sparse prior, we employed the
Bernoulli–Uniform distribution $\phi_{\text{BU}}(w|\rho) = (1-\rho)\delta(w) + \rho$
since we have no prior knowledge about the distribution of
the non-zero components. The hyper-parameter $\rho$ was tuned
to make the expected number of non-zero components in the
posterior distribution correspond to the controlled value
$K(=1, 2, \ldots)$. For each $K$, the other hyper-parameter $\beta$ was determined so that the approximate LOOE [19] was minimized.

To examine the validity of the approximate estimate, we also literally carried out LOO CV, utilizing the same values of hyper-parameters as those of the approximate method. Table I summarizes LOOEs evaluated for $K = 1, 2, \ldots, 6$. The values in the top row were obtained by the approximate CV formula of [19] while those in the middle row were evaluated by literally performing LOO CV. The values are reasonably consistent with each other, which validates the usage of [19]. The bottom row contains the achieved RSS per data for reference.

Table I indicates that LOOEs are minimized around $K = 4$ while the achieved RSS per data decreases monotonically as $K$ grows, which makes it possible to choose the optimal hyper-parameter as $K = 4$ by monitoring the approximate LOOE evaluated by [19]. Figure 2 (a) shows the stem plot of the estimator $m = (m_1)$ obtained for this optimal choice. This indicates that most components except for the variables “1” and “2,” which stand for light curve width and color index, respectively, are negligibly small. That said, variable “233” has the third largest amplitude, and may not be negligible. In fact, this variable is defined by normalizing the spectral intensity of wavelength 6631 Å by the “continuum level” (roughly speaking, a locally smoothed intensity around the wave length), and hardly varies in the data set. This suggests that the possibly non-negligible amplitude may be due to an accidental statistical fluctuation. Indeed, analyzing the same data set enforcing $m_{233} = 0$ produces almost the same profile as in Fig. 2 (a) for other components (Fig. 2 (b)), which implies that $m_{233}$ does not play an important role in the regression. This may indicate that only the light curve width and color index are relevant for estimating the absolute magnitude at the maximum of type Ia supernovae, which is consistent with the conclusions of earlier studies [15], [16].

V. Summary and Discussion

In summary, we developed a semi-analytic formula to evaluate the CV error approximately for Bayesian linear regression. When the Hessian of the EC free energy is available, the formula makes it possible to evaluate approximately the leave-one-out CV error (LOOE) from the full estimator without actually performing CV. The usefulness of the developed formula was tested and confirmed by applications to a synthetic model and a real world data set of type Ia supernovae.

We make two observations: First, although we employed the EC approximation, similar formulas can also be developed in other approximation frameworks such as the naive mean field and the Bethe approximations. Second, the standard linear regression, ridge regression, and LASSO can be formulated as the maximum a posteriori estimator in the Bayesian framework. Techniques similar to that developed in the current paper can reproduce their existing formulas of LOOE by introducing an appropriate $\beta$-dependent prior and letting $\beta \to \infty$. In this sense, the developed formula [19] can be regarded as a generalization of the existing formulas.

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