Stopping Criterion for Active Learning Based on Error Stability

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Abstract

Active learning is a framework for supervised learning to improve the predictive performance by adaptively annotating a small number of samples. To realize efficient active learning, both an acquisition function that determines the next datum and a stopping criterion that determines when to stop learning should be considered. In this study, we propose a stopping criterion based on error stability, which guarantees that the change in generalization error upon adding a new sample is bounded by the annotation cost and can be applied to any Bayesian active learning. We demonstrate that the proposed criterion stops active learning at the appropriate timing for various learning models and real datasets.

Keywords: supervised learning, active learning, stopping criterion, PAC-Bayesian learning

1. Introduction

In supervised learning, increasing the size of the training dataset would improve the predictive accuracy. However, a sufficient number of data often cannot be obtained since the annotation cost is high. Active learning (AL) is a framework for acquiring data to improve the generalization error of a predictor and it is effective when only a small number of data is available (Settles, 2009; Dasgupta, 2011; Hino, 2020). The effectiveness of AL depends on both the acquisition function used for selecting effective data to improve the generalization error of the predictor and the stopping criterion used for determining the stopping timing. However, most conventional AL methods adopt the “fixed budget” approach, which acquires samples until the size of the labeled dataset reaches to a predetermined budget. The fixed budget approach considers only the annotation cost and the generalization error is not considered; hence, it often causes overexploitation or a deficiency. Therefore, a stopping criterion considering the generalization error is required to utilize AL effectively.
The optimal stopping timing of AL is determined subjectively by users since there is a trade-off between decreasing the annotation cost and increasing the performance of the predictor. Therefore, it is essential for a stopping criterion of AL to have the ability to determine whether to aggressively or conservatively stop learning, taking into account the trade-off (Altschuler and Bloodgood, 2019). However, it is not easy for a stopping criterion to satisfy this requirement for the following two reasons. First, it is not easy to evaluate the performance of the predictor in AL. Although the generalization error is estimated by using the test dataset in a standard setting of supervised learning, it is not appropriate for AL, which aims to learn from a small amount of data. Second, it is not easy to compare the annotation cost and performance numerically on the same scale since the units of measurement of the annotation cost and performance are different.

In this study, we propose a stopping criterion based on the upper bound of the change in generalization error upon adding a new sample. The proposed criterion guarantees that the change in generalization error is less than a pre-determined threshold. The change of generalization errors guaranteed by the proposed criterion is normalized with respect to the range of the generalization error. Therefore, the proposed criterion stops learning at a similar timing for any dataset when the same threshold is used. Furthermore, the proposed criterion can be applied to arbitrary Bayesian predictive models. We demonstrate the effectiveness of the proposed criteria for several Bayesian ALs.

The contributions of this study are as follows.

1. **Versatile stopping criteria for Bayesian active learning are proposed.**
   The proposed criterion can be applied to arbitrary Bayesian AL active learning algorithms. The criterion controls the stop timing of AL based on the stability of the generalization error. We experimentally demonstrate that the proposed criterion has a high correlation with the generalization error and its threshold can be determined without depending on the dataset as long as the same learning model is used.

2. **A bound of the difference between generalization errors is proved.**
   We prove that the difference between expected generalization errors with respect to Bayes posteriors can be bounded based on a probably approximately correct (PAC) Bayesian framework. Unlike conventional PAC-Bayesian learning, our bound does not assume independence among samples. In this sense, the bound is suitable for AL. Moreover, we can guarantee that the proposed bound converges to zero when the posterior converges.

3. **The proposed criteria are applied to several Bayesian AL algorithm.**
   In this study, we demonstrate that the proposed criteria can stop the following Bayesian AL algorithms at the appropriate timing: Bayesian linear regression, Bayesian logistic regression, Gaussian process regression, and dropout-based Bayesian deep learning. In particular, we derive analytical expressions for both the Kullback-Leibler (KL) divergence between GP posteriors and the bound of the KL-divergence between posteriors of deep Bayesian learning.

The rest of the paper is organized as follows. Section 2 summarizes the AL framework and the existing measures used for stopping AL algorithms. Section 3 defines the optimal stopping timing. Sections 4 describes the method for automatically stopping AL based on
error stability and another interpretation of the proposed method from the viewpoint of a martingale. Sections 5 demonstrates the effectiveness of the proposed method for four learning models. Section 6 is devoted to conclusions. We note that a preliminary version of this work is presented in (Ishibashi and Hino, 2020).

2. Active learning and its stopping criteria

2.1 Active learning

Let $x \in X$ and $y \in Y$ be an input variable and the corresponding output variable, respectively. The purpose of supervised learning is to estimate a predictor $f : x \mapsto \mathbb{E}[y|x]$ from a training dataset. Active learning is a framework for selecting a small number of datasets, which is useful for improving the generalization error of the predictive model by iterating the following two processes: (i) estimate the predictor from current training data, and (ii) acquire new training data by maximizing an acquisition function. We denote the acquisition function by $g$. Then, the next data is selected as

$$
    x^* = \arg \max_{x \in X} g \left( x \mid f \right).
$$

We note that there are batch active learning methods, but for simplicity, we consider only one sample at a time for annotation. The acquisition functions are classified into two approaches, namely, an informative sample selection approach and a representative sample selection approach (Dasgupta, 2011). The informative sample selection approach selects the most uncertain datum for the predictor (Lewis and Gale, 1994; Scheffer et al., 2001; Yang et al., 2015; Seung et al., 1992; Freund et al., 1992; Houlsby et al., 2011; Kirsch et al., 2019). On the other hand, the representative sample selection approach selects a datum representing the overall input distribution (Nguyen and Smeulders, 2004; Settles and Craven, 2008). These two approaches can be combined to achieve the optimal acquisition function (Xu et al., 2003; Donmez et al., 2007; Huang et al., 2010; Karzand and Nowak, 2020). Recently, as another approach, methods of learning acquisition functions have also been proposed (Konyushkova et al., 2017; Sener and Savarese, 2018; Taguchi et al., 2021).

2.2 Conventional stopping criteria for active learning

Most active learning methods adopt the fixed-budget approach, which stops learning when the number of annotated data reaches a predetermined size. However, this approach tends to cause undersampling or oversampling since it is rare to know the appropriate sampling size for satisfactory prediction accuracy in advance. While the predictor may be useless because of the lack of generalization error in the case of undersampling, the efficient sampling in AL may be wasted in the case of oversampling. Therefore, a stopping criterion considering the generalization error is required.

The conventional stopping criterion for AL can be classified into three approaches: accuracy-based, confidence-based and stability-based approaches. In the accuracy-based approach, predictive error is evaluated by using unlabeled or past training data. A typical method is to evaluate the predictive error by using queried or selected unlabeled data (Zhu, 2007; Zhu et al., 2008a, b; Laws and Schütze, 2008). In the confidence-based approach,
the stopping timing is determined by the confidence of prediction with respect to unla-
beled data. For example, the margin of a support vector machine (SVM), entropy, mutual
information or the agreement of learners is used for evaluating uncertainty (Schohn and
Cohn, 2000; Vlachos, 2008; Zhu, 2007; Krause and Guestrin, 2007; Tomanek et al., 2007;
Olsson and Tomanek, 2009). In the stability-based approach, active learning is stopped by
evaluating the difference between values before and after obtaining a new training datum.
Stopping criteria based on stability such as the parameter change given new data, the agree-
ment between the most recent learner and the previous learner and the predicted change
in F-measure have been proposed (Bloodgood and Vijay-Shanker, 2009; Bloodgood and
Grothendieck, 2013; Altschuler and Bloodgood, 2019). However, except for a small number
of methods (Krause and Guestrin, 2007; Bloodgood and Grothendieck, 2013; Altschuler
and Bloodgood, 2019), most of these methods lack theoretical underpinning. Moreover,
the stopping criterion proposed by Krause and Guestrin (2007) assumes Gaussian process
regression as a predictive model and it is necessary to discretize the domain of explanatory
variables. The criteria proposed by Bloodgood and Grothendieck (2013) and Altschuler
and Bloodgood (2019) can be applied to any classification model but not to regression models.

Theoretically, a stopping criterion for disagreement-based active learning (Balcan et al.,
2009; Hanneke, 2014) could be applicable to wide variety of learning models. It is also
equipped with a learning-theoretical stopping criterion. However, it is difficult to apply
disagreement-based active learning to practical problems.

2.3 PAC-Bayesian learning

As another approach, we can consider terminating active learning by using PAC-Bayesian
learning. Let $D$ be the true distribution for a pair of input variable $x \in X$ and its corre-
sponding output variable $y \in Y$. We assume that a training dataset $S = \{(x_i, y_i)\}_{i=1}^{n}$ is
generated by $D$. We specify the dataset at time $t$ in AL as $S_t$, which is the union of the
initial dataset $S_0 = \{(x_i, y_i)\}_{i=1}^{n_0}$ and the acquired dataset $\{(x_i, y_i)\}_{i=1}^{n_t}$, and the size of $S_t$
is denoted by $n_t$. Denoting a predictor parameterized by $\theta$ as $f_{\theta}$, we respectively define the
training and generalization errors for $f_{\theta}$ as

$$
\hat{L}(\theta) := \frac{1}{n} \sum_{i=1}^{n} l(f_{\theta}(x_i), y_i), \quad L(\theta) := \mathbb{E}_D [l(f_{\theta}(x), y)]
$$

where $l(f_{\theta}(x), y) \in [a, b]$ is the loss function for the predictor. Let $p(\theta|S)$ be a Bayesian
posterior distribution given $S$. In the PAC-Bayesian learning framework (McAllester, 1999;
Guedj, 2019; Germain et al., 2016), we consider evaluating the upper bound of the ex-
pectation of the generalization error with respect to the Bayesian posterior by using the
expectation of the training error and the Kullback–Leibler (KL) divergence between the
posterior and the prior (McAllester, 1999). For example, let the expected training error
and generalization error with respect to the Bayesian posterior $p(\theta|S)$ be

$$
\hat{L}(p(\theta|S)) := \mathbb{E}_{p(\theta|S)} [\hat{L}(\theta)], \quad L(p(\theta|S)) := \mathbb{E}_{p(\theta|S)} [L(f)],
$$

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and the KL-divergence is defined as $D_{KL} [p(\theta)||q(\theta)] := \mathbb{E}_{p(\theta)} [\log p(\theta)/q(\theta)]$. Then, McAllester (1999) proved that the following bound holds with probability at least $1 - \delta$:

$$L(p(\theta|S)) \leq \hat{L}(p(\theta|S)) + \sqrt{D_{KL} [p(\theta|S)||p(\theta)] + \log \frac{2\sqrt{n}}{\delta}},$$

where $p(\theta)$ is any prior probability distribution independent of $S$. This bound is only applicable to classification problems, but several bounds for regression problems have been considered by Germain et al. (2016).

PAC-Bayesian bounds are promising tools for developing a stopping criterion for active learning, but conventional PAC-Bayesian bounds suffer the following two drawbacks. First, most of the PAC-Bayesian bounds assume that samples are realizations of i.i.d. random variables. This assumption is not suitable for active learning since a new sample depends on previous data samples. PAC-Bayesian bounds for non-i.i.d. samples have been proposed (Alquier and Guedj, 2018; Seldin et al., 2012). These approaches assume that the difference between the generalization error and the training error follows $\alpha$-mixing or a martingale, but it is not trivial to apply them to an AL. Therefore, to the best of our knowledge, there is no suitable PAC-Bayesian bound for active learning. Second, it is difficult to determine a suitable threshold for stopping AL because the expected generalization error depends on the dataset and model. This makes it difficult for users to set an appropriate parameter for the dataset at hand. It is also important, depending on the application, to stop active learning rapidly without waiting the convergence of learning or to stop learning once confident of convergence of the generalization error.

In this study, we propose a stopping criterion based on the error stability of the expected generalization error. The proposed criterion does not require any assumption with respect to models like PAC-Bayesian learning. On the other hand, the proposed criterion does not assume that samples are i.i.d. random variables, unlike PAC-Bayesian learning. Furthermore, it is easy to determine a threshold of the proposed criterion, since the range of the threshold is restricted to $[0,1]$ for any dataset.

3. Definition of optimal stopping timing based on error stability

We denote the posterior given $S_t$ by $p(\theta|S_t)$, where $S_t$ is the training dataset at time $t$ in active learning. Let $\mathcal{L}(\theta) \in [a,b]$ be the generalization error for $\theta$ and $\mathbb{E}_{p(\theta|S_t)} [\mathcal{L}(\theta)]$ be the expected generalization error for the posterior. Assuming that the sampling cost is constant $\kappa \in [0,\infty)$, the standard definition of the optimal stopping timing is

$$t^* := \arg \min_t \left\{ \mathbb{E}_{p(\theta|S_t)} [\mathcal{L}(\theta)] + \kappa t \right\},$$

which balances the expected generalization error and sampling cost. However, it is impossible to obtain $t^*$ for the following two reasons. First, it is difficult to calculate the first term of Eq. (1) since it is not realistic to estimate the generalization error by using a test dataset in active learning problems. Second, it is not easy to know the appropriate sampling cost $\kappa$ in a comparable unit to the generalization error.
In this study, we consider estimating the optimal stopping timing by using the difference between the generalization errors before and after obtaining a new training datum, which is denoted by
\[ \Delta L_i := E_p(\theta|S_i)[L(\theta)] - E_p(\theta|S_{i-1})[L(\theta)]. \]
Note that \( E_p(\theta|S_0)[L(\theta)] \) is a constant; thus, the following equation holds:
\[
t^* = \arg\min_t \left\{ E_{p(\theta|S_t)}[L(\theta)] + \kappa t \right\}
= \arg\min_t \left\{ \frac{1}{\gamma} \sum_{i=1}^{t} \Delta L_i + \frac{\kappa}{\gamma} t \right\},
\]
where \( \gamma \) is a parameter used to normalize the range of \( \lambda := \kappa/\gamma \) to [0, 1]. The optimal stopping timing is equal to the timing satisfying \( \Delta L_i/\gamma \leq \lambda \) when the first derivative of \( E_{p(\theta|S_t)}[L(\theta)] \) is a monotonically decreasing function, but this does not hold in general. Therefore, instead of assuming the condition, we suppose that \( \Delta L_i \) gradually decreases with time. Then, the above optimal stopping timing can be approximated as
\[
t^* \approx \min_t \left\{ t > 0 \left| \frac{\Delta L_t}{\gamma} \leq \lambda \right. \right\}.
\]
With this definition, we can stop active learning at the optimal stopping timing by monitoring \( |\Delta L_t|/\gamma \) in the sequential process of adding a new sample and updating the predictive model. Since the condition \( |\Delta L_t| \leq \kappa \) is called error stability in Bousquet and Elisseeff (2002), we call the stopping criterion based on Eq. (3) the error stability based stopping criterion. We note that in the above formulation, there is no need to determine the sampling cost \( \kappa \). Instead, we have to set the threshold \( \lambda \), which should be easier than determining the sampling cost for each model and dataset because the range of the threshold is restricted to [0, 1] and it has an intuitive interpretation as explained in the next section.

4. Stopping criterion based on error stability

The error stability based criterion in Eq. (3) contains the difference in generalization error \( \Delta L_t \), which is not directly available. In this section, we derive the upper bound of \( \Delta L_t \), estimable by using the posterior distribution of Bayesian predictive models.

4.1 Proposed stopping criterion

In this study, we consider Bayesian predictive models. Let \( p(\theta) \) and \( p(\theta|S) \) respectively be the prior and posterior distributions given a set of observations \( S \) defined as
\[
p(\theta|S) = \frac{1}{Z} \exp\{ -\rho \hat{L}(\theta) \} p(\theta),
\]
where \( \rho \geq 0 \) is a parameter controlling the trade-off between training error and the prior and \( Z \) is the normalization constant corresponds to the Bayesian marginal likelihood. Then, the following theorem holds:
Then, by using Theorem 1, the upper bound of \(|\Delta \mathcal{L}|/\gamma\) is derived as

$$\frac{|\Delta \mathcal{L}_t|}{\gamma} \leq \frac{(b-a)r_t}{\gamma}.$$  

To remove the range \((b-a)\) from the upper bound, we define \(\gamma = (b-a)\hat{\gamma}\). In this study, as shown in Fig. 1, we propose to stop active learning when the following condition holds:

$$\lambda_t := \frac{r_t}{\hat{\gamma}} \leq \lambda,$$  

\hline

1. More generally, for any \(v \geq \mathbb{E}[\mathcal{L}^2(\theta)]\), the following inequality holds:

$$-\frac{v}{b-a}(\exp\{W_0(u') + 1\} - 1) \leq \mathbb{E}_{p(\theta|S')} [\mathcal{L}(\theta)] - \mathbb{E}_{p(\theta|S')} [\mathcal{L}(\theta)] \leq -\frac{v}{b-a}(\exp\{W_0(u) + 1\} - 1),$$

where \(u' := ((b-a)^2D_{\mathcal{KL}}[p(\theta|S')||p(\theta|S)] - v)/ve\) and \(u := ((b-a)^2D_{\mathcal{KL}}[p(\theta|S)||p(\theta|S')] - v)/ve\).
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Algorithm 1  Error stability based stopping criterion

\begin{algorithmic}
\STATE Input $\lambda > 0$, $S_0$, $\tilde{\gamma}$
\STATE $t \leftarrow 0$
\STATE $p_t(\theta) \leftarrow \frac{1}{Z} \exp\{-\rho \tilde{L}(\theta)\} p(\theta)$
\STATE $\tilde{\lambda}_t \leftarrow 1$
\WHILE{$\lambda < \lambda_t$}
\STATE $x_t = \arg \max_{x \in X} g(x|\theta)$
\STATE $S_t \leftarrow S_{t-1} \cup \{(x_t, y_t)\}$
\STATE $p_t(\theta) \leftarrow \frac{1}{Z} \exp\{-\rho \tilde{L}(\theta)\} p(\theta)$
\STATE $r(p_t, p_{t-1}) \leftarrow \exp\left\{W_0 \left(\frac{D_{KL}[p_t(\theta)\|p_{t-1}(\theta)]}{e} - 1\right) + 1\right\} - 1$
\STATE $r(p_{t-1}, p_t) \leftarrow \exp\left\{W_0 \left(\frac{D_{KL}[p_{t-1}(\theta)\|p_t(\theta)]}{e} - 1\right) + 1\right\} - 1$
\STATE $\lambda_t \leftarrow r(p_t, p_{t-1}) + r(p_{t-1}, p_t)/\tilde{\gamma}$
\ENDWHILE
\end{algorithmic}

where the error stability is guaranteed to satisfy $|\Delta L_t|/(b-a)\tilde{\gamma} \leq \lambda$. When $r_t$ is larger than $r_1$, it is not less than the threshold; hence, we choose $\tilde{\gamma} = r_1$ in order to ensure that the range of $\lambda$ is $[0,1]$ and call $\lambda_t$ the “error ratio”\footnote{In practice, since $r_1$ can be extremely larger than the other $r_t, t > 1$, the learning process may stop before the convergence of generalization error when $\tilde{\gamma} = r_1$. To avoid this problem, we iterate at least 10 acquisitions and set $\tilde{\gamma} = \min\{r_t\}_{t=1}^m$, where $m = 1$ for experiments with a Bayesian deep neural network model, and $m = 10$ with other models in our implementation.}. The concrete algorithm is shown in Algorithm 1.

The proposed criterion has three favorable properties. First, the proposed criterion does not require any assumption including independence between samples. This is suitable for an active learning framework, since acquired samples affect the selection of the next sample. Second, $\lambda_t$ goes to zero because $W_0(-1/e) = -1$ holds when the KL-divergence becomes zero. Therefore, the proposed criterion guarantees that after observing a sufficient number of samples, the active learning is terminated. Finally, the proposed criterion is based on the upper bound of the gap between the normalized generalization errors without specifying the range of the generalization error. This is a major advantage of the proposed criterion because, in general, it is difficult to know the range of the generalization error in advance.

Remark 2 \textit{In this paper, to apply AL, we explain the proposed bound as the bound for the gap between expected generalization errors with respect to Bayes posteriors. However, Theorem 1 can be applied to any measurable function and any probability density function.}

4.2 Interpretation of the proposed stopping criterion from the viewpoint of martingale theory

The proposed criterion can be interpreted from the viewpoint of martingale theory. Denoting the expected generalization error with respect to the posterior distribution $q_t(\theta)$ by $E_t$, we consider the sequence $E_1^t = \{E_1, E_2, \ldots, E_t\}$. Then, the following theorem holds:
Theorem 3 The sequence $E^t_1$ is assumed to be a supermartingale, namely, $\mathbb{E}[E_i|E_{i-1}^t] \leq E_{i-1}$. For any $0 < \eta < 1$ and $0 < \delta < 1$ satisfying

$$\lambda_t \leq \sqrt{-\frac{2}{\log(\delta/2)}} \eta = \lambda,$$

the following inequality holds with probability at least $1 - \delta$:

$$|E_t - \mathbb{E}[E_t|E_{t-1}^t]| \leq (b - a) \gamma \eta.$$

Proof See Appendix A. □

$\mathbb{E}[E_i|E_{i-1}^t]$ is the conditional expectation of the expected generalization error $E_i$ with respect to a new sample generated by random sampling given $E_{i-1}^t$. We can conclude that the stopping criterion guarantees the effectiveness of active learning since $E_i - \mathbb{E}[E_i|E_{i-1}^t] < 0$ indicates that the expected generalization error by using AL is larger than the conditional expectation of the expected generalization error.

5. Experimental results

In this section, the versatility of the proposed criterion is demonstrated through active learning experiments using datasets from the UCI machine learning repository (Dua and Graff, 2017). As Bayesian active learners, four AL models are considered: Bayesian ridge regression (BRR), Bayesian logistic regression (BLR), Gaussian process regression (GPR) and Bayesian deep neural network (BDNNs). A description of the datasets is given in Table 1. Every feature of these datasets is normalized to have zero mean and a standard deviation of one.

| Name of dataset             | Sample size | Feature dimension | Test size | AL model   |
|----------------------------|-------------|-------------------|-----------|------------|
| Power plant                | 9568        | 4                 | 2000      | BRR, GPR   |
| Protein                    | 45730       | 9                 | 2000      | BRR, GPR   |
| Gas emission               | 36733       | 8                 | 2000      | BRR, GPR   |
| Grid stability for regression | 10000     | 11                | 2000      | BRR, GPR   |
| Grid stability for classification | 10000   | 11                | 5000      | BLR        |
| Skin                       | 245057      | 3                 | 5000      | BLR        |
| HTRU2                      | 17897       | 7                 | 5000      | BLR        |
| MNIST                      | 70000       | 784               | 10000     | BDNNs      |

5.1 Evaluation measure

It is difficult to evaluate the effectiveness of the stopping timing because of the lack of a subjective, ground truth optimal stopping timing. In fact, the appropriate threshold to
stop learning should be problem-dependent. The proposed stopping criterion is based on
the estimate of the upper bound of the generalization error. To demonstrate the validity
of the proposed method, we evaluate the correlation coefficient between the error ratio
and the expected generalization error, which is estimated by using a sufficient number
of test data. When the error ratio is highly correlated with the expected generalization
error, it provides additional evidence that our proposed method is suitable for stopping
active learning based on the expected generalization error. Let
\[
E^t_1 = \{E_1, E_2, \ldots, E_t\}
\]
and
\[
\Lambda^t_1 = \{\lambda_1, \lambda_2, \ldots, \lambda_t\}
\]
be sequences of expected generalization errors and error ratios, respectively. Since
\(\lambda_t\) satisfying \(\lambda_t \neq \min \Lambda^t_1\) does not affect the stopping timing of AL, we
evaluate the correlation between the following two sets:
\[
\hat{E}^t_1 = \{E_i | i = \arg \min \Lambda^t_i, \quad i \in \{1, 2, \ldots, t\}\},
\]
\[
\hat{\Lambda}^t_1 = \{\lambda_i | i = \arg \min \Lambda^t_i, \quad i \in \{1, 2, \ldots, t\}\}.
\]
The form of the likelihood function is highly dependent on the predictive model, and the
appropriate threshold will be different for different models. However, when we use the same
predictive model, regardless of the dataset, it is desirable that the same threshold results in
approximately the same stopping timing in terms of the convergence of the generalization
error. In this experiment, we verify that the proposed criterion stops AL at about the
same timing for various datasets when the learning model is fixed. We set thresholds
\(\lambda = 0.02, 0.015, 0.01\) for BRR; \(\lambda = 0.3, 0.2, 0.1\) for BLR; \(\lambda = 0.05, 0.04, 0.03\) for GPR; and
\(\lambda = 0.2, 0.15, 0.1\) for BDNNs.

5.2 Active learning models
We consider the following four active learning models:

1. Bayesian ridge regression
In BRR, the predictor \(f : \mathcal{X} \to \mathcal{Y}\) is modeled by a linear combination of \(J\) basis functions,
\(\psi = (\psi_1, \psi_2, \ldots, \psi_J)^T\), that is,
\[
f(x) = w^T \psi(x),
\]
where \(w \in \mathbb{R}^J\). We assume that the likelihood function \(p(y|w, x)\) given \(S\) and the prior
distribution \(p(w)\) for parameter \(w\) are written as
\[
p(y|w) = \prod_{i=1}^{n} \mathcal{N}(y_i|w^T \psi(x_i), \beta^{-1}),
\]
\[
p(w) = \mathcal{N}(w|0, \alpha^{-1}I),
\]
where \(y = (y_1, y_2, \ldots, y_n)^T\), \(\beta\) is the accuracy of Gaussian noise and \(\alpha\) is the accuracy of
the prior. Let \(\Psi = (\psi(x_1), \psi(x_2), \ldots, \psi(x_n))\) be the matrix of feature vectors. Then, the
posterior of parameter \(w\) is derived as
\[
p(w|S) = \mathcal{N}(w|\mu, \Sigma),
\]
\[
\mu = \beta \Sigma \Psi \bar{y},
\]
\[
\Sigma^{-1} = \beta \Psi \Psi^T + \alpha I.
\]
We define the acquisition function of BRR by the variance of the predictive distribution
\[ g(x) = \psi^T(x) \Sigma \psi(x). \]

To apply the proposed criterion, we have to calculate the KL-divergence between \( p(w|S) = \mathcal{N}(w|\mu, \Sigma) \) and \( p(w|S') = \mathcal{N}(w|\mu', \Sigma') \). In BRR, since the posterior becomes a normal distribution, the KL-divergence is explicitly written as
\[
D_{KL} [p(w|S')||p(w|S)] = \frac{1}{2} \left\{ \text{Tr}[\Sigma^{-1} \Sigma'] - \log \Sigma^{-1} \Sigma' + (\mu - \mu')^T \Sigma^{-1} (\mu - \mu') - J \right\}.
\]

In this experiment, we use the additive model for radial basis function (RBF) bases to define the predictor \( f \) as
\[
f(x) = \sum_{d=1}^{D} \sum_{m=1}^{M} w_{md} \psi_{md}(x),
\]
where \( \psi_{md}(x) \) is the \( d \)th dimension of the \( m \)th basis,
\[
\psi_{md}(x) = \exp \left( -\frac{1}{2l^2} (x_d - \xi_m)^2 \right).
\]
The \( M \) centers of bases \( \xi_m \) are common for all dimensions and are arranged at equal intervals in the range of the observed explanatory variables. The bandwidth parameter \( l \) is set to be \( l = \Delta_\xi \), where \( \Delta_\xi \) is the length between adjacent centers \( \xi_m \). The hyperparameters \( \alpha \) and \( \beta \) are estimated by maximizing the marginal likelihood with the training dataset, that is, by solving the following self-consistent equations:
\[
\alpha = \frac{\tau}{\mu^T \mu}, \quad \frac{1}{\beta} = \frac{1}{N_T - \tau} (y - \mu^T \Psi)^2,
\]
where \( \tau = \sum_i \tau_i / (\tau_i + \alpha) \) with the \( i \)th eigenvalue \( \tau_i \) of the matrix \( \beta \Psi^T \Psi \).

2. Bayesian logistic regression
BLR considers the two-class classification problem. When \( S \) is observed, the predictor \( p(y = 1|x) \) is modeled by using a linear combination of \( J \) basis functions and the logistic function \( \sigma(a) = 1/(1 + \exp(-a)) \) as
\[
p(y = 1|x) = \sigma(w^T \psi(x)).
\]
The likelihood function and the prior distribution of \( w \) are respectively assumed to have the following forms:
\[
p(y|w) = \prod_{i=1}^{t} \text{Bern}(y_i|p_i),
\]
\[
p(w) = \mathcal{N}(w|0, \alpha^{-1} I),
\]
where \( \alpha \) is the accuracy of the prior. Since the posterior distribution of the Bayesian logistic regression model does not have a closed-form representation, we use the Laplace approximation as
\[
p(w|S) \approx \mathcal{N}(w|w_{MAP}, H), \tag{6}
\]
where $w_{\text{MAP}}$ is the MAP estimate of the posterior and $H$ is the Fisher information matrix for the posterior at $w_{\text{MAP}}$. We use the entropy of the predictor as the acquisition function:

$$g(x) = -\sum_{c \in \{0,1\}} p(y = c|x) \log p(y = c|x).$$

It is easy to calculate the KL-divergence for BLR since the posterior is a normal distribution. From Eq. (6), the KL-divergence between $p(w|S) \approx N(w|w_{\text{MAP}},H)$ and $p(w|S') \approx N(w|w'_{\text{MAP}},H')$ is derived as

$$D_{\text{KL}} [p(w|S')||p(w|S)] = \frac{1}{2} \left\{ \text{Tr}[H^{-1}H'] - \log H^{-1}H' + (w_{\text{MAP}} - w'_{\text{MAP}})^T H^{-1} (w_{\text{MAP}} - w'_{\text{MAP}}) - J \right\}.$$

We use the additive model of RBF bases and adopt the same basis functions as for BRR.

3. Gaussian process regression

Let $S$ be the observed dataset. In Gaussian process regression, the loss function is assumed to be the negative log likelihood of the Gaussian distribution with accuracy $\beta$, and the prior distribution is obtained as

$$\begin{bmatrix} y \\ f(x) \end{bmatrix} \sim N\left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K + \beta^{-1}I & k(x) \\ k^T(x) & k(x,x) \end{bmatrix} \right),$$

where $k(x,x)$ is the kernel function, $k(x) = k(X,x)$, $K = k(X,X)$, $X = \{x_1, x_2, \ldots, x_n\}$ and $y = (y_1, y_2, \ldots, y_n)$. Then, the posterior is defined as

$$f(x)|x, S \sim N(\mu(x), \sigma(x,x)),$$

where $\mu(x) = k^T(x)(K + \beta^{-1}I)^{-1}y$ and $\sigma(x,x) = k(x,x) - k^T(x)(K + \beta^{-1}I)^{-1}k(x)$. We adopt the variance of the predictive distribution as the acquisition function:

$$g(x) = k(x,x) - k^T(x)(K + \beta^{-1}I)^{-1}k(x).$$

It is not easy to calculate the KL-divergence between GP posteriors since the KL-divergence diverges to infinity in general, but it is computable when the prior of the GP posteriors is fixed. Let $q(f|S_t)$ and $q(f|S_{t-1})$ be the posteriors of $f$ given $S_t$ and $S_{t-1}$, respectively. Then, the following equalities hold:

$$D_{\text{KL}} [p(f|S_{t-1})||p(f|S_t)] = \frac{1}{2} \beta \sigma_{t-1}(x_{n_t}, x_{n_t}) - \frac{1}{2} \log (1 + \beta \sigma_{t-1}(x_{n_t}, x_{n_t})) + \frac{1}{2} \beta \sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1} (y_{n_t} - \mu_{t-1}(x_{n_t}))^2,$$

$$D_{\text{KL}} [p(f|S_t)||p(f|S_{t-1})] = \frac{1}{2} \log (1 + \beta \sigma_{t-1}(x_{n_t}, x_{n_t})) - \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1} \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1} (y_{n_t} - \mu_{t-1}(x_{n_t}))^2.$$

Details of the derivation are described in Appendix B.
In this study, the kernel function for the prior is the following Gaussian kernel:

$$k(x, x') = \exp \left( -\frac{1}{2l^2} \|x - x'\|^2 \right).$$

The hyperparameters $l$ and $\beta$ are chosen by maximizing the marginal likelihood with training data.

4. Dropout-based Bayesian deep learning

We consider the dropout-based BDNNs of $L$-layer perceptron (Gal and Ghahramani, 2016), where the $l$th layer has $H_l$ neurons composed of a weight vector denoted by $W_l \in \mathbb{R}^{H_l \times H_{l-1}}$ and a bias denoted by $b_l \in \mathbb{R}^{H_l}$. The 0th layer is the input layer and $H_0$ is the number of its neurons. In each epoch during the training, several elements of the weight vectors of the dropout-based BDNNs model are randomly set to zero. The dropped out weight vectors of the $l$th layer are described as $W_l = M_l \text{diag}(e_{lh})_{h=1}^{H_l-1}$, where $e_{lh} \sim \text{Bern}(p_l)$.

Let $\sigma_l : \mathbb{R}^{H_{l-1}} \rightarrow \mathbb{R}^{H_l}$ be the $l$th layer’s activation function. The output of the $l$th layer is described as $z_l = \sqrt{\frac{1}{H_l}} \sigma_l(W_l z_{l-1} + b_l)$, where $z_{l-1}$ is the $(l - 1)$th layer’s output and $z_0$ is the input vector $x \in X$. Therefore, the predictor is modeled as $f(x) = \sqrt{\frac{1}{H_L}} \sigma_L(W_L z_L + b_L)$.

As the acquisition function, we use batchBALD (Kirsch et al., 2019), which is an extension of BALD (Houlsby et al., 2011), to select multiple points simultaneously. It uses the mutual information $I(y; \theta|S, x)$ between the output $y$ for the input $x$ given training data $S$ and model parameter $\theta$.

Let $\theta$ be the whole parameter of the model. We assume that the prior is $p(\theta) = \prod_{l=1}^{L} \prod_{h=1}^{H_{l-1}} p(w_{lh})p(b_l)$, where $p(w_{lh}) = p(b_l) = \mathcal{N}(0, I)$. The posterior probability $q(\theta)$ is, by using the mean field approximation, written as the product of marginals:

$$q(\theta) = \prod_{l=1}^{L} p(W_l)p(b_l).$$

In this formula,

$$q(W_l) = \prod_{h=1}^{H_{l-1}} q(w_{lh}), \quad q(b_l) = \mathcal{N}(\nu_l, \sigma_l^2 I)$$

and

$$q(w_{lh}) = p_l \mathcal{N}(m_{lh}, \sigma_l^2 I) + (1 - p_l) \mathcal{N}(0, \sigma_l^2 I).$$

Hence $q(\theta)$ is shown to be a mixture of Gaussians.

The analytical formula for the KL-divergence between mixture distributions is not known, but its upper bound can be derived by using the chain rule for the KL-divergence (Do, 2003; Hershey and Olsen, 2007). Let $p(\theta) = \sum_{k=1}^{K} \pi_k p_k(\theta)$ and $q(\theta) = \sum_{k=1}^{K} \omega_k q_k(\theta)$ be any
Gaussian mixture models with $K$ components. The KL-divergence between $p(\theta)$ and $q(\theta)$ is bounded as

$$D_{\text{KL}}[p(\theta)\|q(\theta)] \leq \sum_{k=1}^{K} \pi_k \left[ D_{\text{KL}}[p_k(\theta)\|q_k(\theta)] + \log \frac{\pi_k}{\omega_k} \right],$$

By using this bound, the following inequality is derived:

$$D_{\text{KL}}[p(\theta)\|q(\theta)] \leq \frac{1}{2} \sum_{l=1}^{L} \left\{ p_l \|M_l - M'_l\|^2_F + \frac{1}{\sigma^2_l} \|\nu_l - \nu'_l\|^2 \right. + \left. H_{l-1}D_{\text{KL}}[p_l\|q_l] \right\}$$

$$+ \sum_{l=1}^{L} (1 + p_l H_{l-1}) H_l \left\{ \frac{\sigma^2_l}{\sigma^2_{l'}} - \log \frac{\sigma^2_l}{\sigma^2_{l'}} - 1 \right\},$$

where $M_l = (m_{l1}, m_{l2}, \ldots, m_{lH_{l-1}})$. We assume that $\sigma^2_l = \sigma^2_{l'}$ and $p_l = p_{l'}$ for any $l \neq l'$. Then, the above inequality is reduced to

$$D_{\text{KL}}[p(\theta)\|q(\theta)] \leq \sum_{l=1}^{L} \frac{1}{2\sigma^2_l} \left\{ p_l \|M_l - M'_l\|^2_F + \|\nu_l - \nu'_l\|^2 \right\},$$

which is a weighted sum of the estimated weight matrices and the squared error of the bias. A detailed derivation is given in Appendix C.

### 5.3 Results

Figure 2 and 3 show correlation coefficients and scatter plots between the expected generalization error and the error ratio defined by Eq. (5), respectively. The correlation coefficients
are greater than 0.9 except for BLR applied to the HTRU2 data. Fig. 6(c) indicates that the expected generalization error increases in the latter half of training in active learning. This is known as the “less is more” phenomenon (Schohn and Cohn, 2000). Since the error ratio bounds the absolute value of the difference between generalization errors, we cannot distinguish whether the difference is positive or negative. Hence, the error ratio has a high correlation with the generalization error, except in the case where the “less is more” phenomenon occurs. Even in such cases, the error ratio correlates with the generalization error until the generalization error starts to increase as shown in Fig. 3(k).

The expected generalization errors evaluated by using the test data and the stopping timings determined by using the proposed criterion with each threshold for each model are shown in Fig. 4, Fig. 5, Fig. 6 and Fig. 7. From Fig. 4 and Fig. 5, the proposed method tends to terminate active learning at about the same timing for any dataset for GPR and BRR when using the same threshold. As shown in Fig. 6, the “less is more” phenomenon is occurred in Power plant and Gas emission for BLR. Thus, the optimal stopping timing is the timing minimizing the generalization error or earlier. As shown in Figs. 3(i)–(k), the threshold of the proposed criterion corresponding to the timing minimizing the generalization error depends on the dataset. Therefore, the proposed criterion with a threshold cannot always stop active learning at the optimal stopping timing, but it can stop it at a reasonably good timing as shown in Fig. 6. From Fig. 7(a), while the proposed method stops active learning when the threshold is 0.2, the proposed method cannot stop active learning when the thresholds are 0.15 and 0.1. This is due to the fact that the proposed criterion converges to around 0.2 as shown in Fig. 7(b). Therefore, we cannot guarantee that the proposed criterion stops active learning when the threshold of the proposed criterion approaches zero for BDNNs, unlike for the other models. However, as long as the threshold is set to be large, we can stop active learning at an appropriate timing for BDNNs.

It is shown that the error ratio has a high correlation with the generalization error for various datasets and AL models, and does not depend on the dataset.

6. Conclusion

In this study, we proposed a stopping criterion for active learning based on error stability. The proposed measure of error stability, i.e., the error ratio, can be applied to any posterior distribution like PAC-Bayesian learning. Unlike the conventional PAC-Bayesian approach, the error ratio does not require any assumption including independence between samples. Furthermore, it is easy to determine the threshold for the proposed criterion, since the range of the threshold is normalized to [0, 1] for any dataset. Moreover, to apply the proposed criterion to Gaussian process regression and Bayesian deep neural networks, we derived analytical expressions for both the KL-divergence between GP posteriors and the upper bound of the KL-divergence between the posteriors of dropout-based Bayesian deep neural networks.

In the experiments, to demonstrate that the proposed criterion can be widely applied to various active learning methods, we applied the criterion to the following four models: Bayesian ridge regression, Bayesian logistic regression, Gaussian process regression and Bayesian deep neural networks. We demonstrated that the error ratio has a high correlation with the generalization error except in the case where the “less is more” phenomenon occurs.
Furthermore, we also demonstrated that the proposed criterion can stop learning at similar timings for various datasets when the same threshold is used.

Although we have explained the proposed bound as the bound for the gap between expected generalization errors with respect to Bayes posteriors, Theorem 1 can be applied to any measurable function and any probability density function. It is expected that the bound will be applied to stop various online learning algorithms such as Bayesian optimization, reinforcement learning and the multi-armed bandit. The applicability of the derived bound to other learning frameworks is an important future work.

**Appendix A. Proof of Theorem 1 and 3**

We demonstrate the following two lemmas to prove Theorem 1.
Figure 4: Expected generalization error and stopping timing for GPR.

Figure 5: Generalization error and stopping timing for BRR.
Lemma 4 (Donsker and Varadhan (1975); McAllester (2003)) Let \( h : \Theta \to \mathbb{R} \) be any measurable function. Then, the following inequality holds:

\[
\mathbb{E}_{p(\theta)} \left[ h(\theta) \right] \leq D_{\text{KL}} \left[ p(\theta) \parallel p'(\theta) \right] + \log \mathbb{E}_{p'(\theta)} \left[ e^{h(\theta)} \right].
\]

Here, \( p \) and \( p' \) are probability distributions on \( \Theta \).

Lemma 5 (Boucheron et al. (2013)) Let \( X_1, X_2, \ldots, X_t \) be independent random variables with \( 0 \leq X_i \leq b, \ b > 0 \), let \( \nu \geq \mathbb{E}[X_i^2] \), and define \( \phi(\lambda) := e^\lambda - \lambda - 1 \). For any \( \lambda > 0 \), the
following inequality holds:

\[
\sum_{i=1}^{t} (\log E[e^{\lambda X_i}] - \lambda E[X_i]) \leq \frac{v}{b^2} \phi(\lambda b).
\]

**Proof of Theorem 1** We denote a difference between \(E_{q(\theta|S)}[L(\theta)]\) and \(E_{q(\theta|S')}[L(\theta)]\) by \(R(q(\theta|S), q(\theta|S'))\). Supposing that \(\tilde{L}(\theta) := L(\theta) - a\), the range of \(\tilde{L}\) is \([0, b']\), where \(b' = b - a\). From Lemma 4 and 5, for any \(s > 0\) we can prove the following inequality:

\[
\begin{align*}
\frac{1}{s} R(q(\theta|S), q(\theta|S')) &= \frac{1}{s} D_{KL} [q(\theta|S)||q(\theta|S')] + \frac{v}{sb'^2} \phi(s b') \\
&\leq D_{KL} [q(\theta|S)||q(\theta|S')] + \frac{v}{sb'^2} \phi(s b').
\end{align*}
\]

This implies

\[
R(q(\theta|S), q(\theta|S')) \leq \frac{1}{s} D_{KL} [q(\theta|S)||q(\theta|S')] + \frac{v}{sb'^2} \phi(s b'), \tag{7}
\]

and \(\partial R/\partial s\) is explicitly written as

\[
\frac{\partial R}{\partial s} = \frac{\partial}{\partial s} \left( v \phi(s b') + b'^2 D_{KL} \right) \\
= \frac{b'^2}{s b'^2} \left( v b'^2 e^{s b'} - v e^{s b'} - (b'^2 D_{KL}) b'^2 \right) \\
= \frac{v s b'^2 e^{s b'} - v e^{s b'} + v - b'^2 D_{KL}}{s^2 b'^2},
\]

where \(D_{KL} := D_{KL} [q(\theta|S)||q(\theta|S')]\). Then, equating \(\partial R/\partial s\) to zero, we obtain

\[
\frac{\partial R}{\partial s} = \frac{v s b'^2 e^{s b'} - v e^{s b'} + v - b'^2 D_{KL}}{s^2 b'^2} = 0 \tag{8}
\]

\[
(s b' - 1) e^{s b'} - 1 = \frac{b'^2 D_{KL} - v}{v e} \tag{9}
\]

\[
\frac{b'^2 D_{KL} - v}{v e} = W \left( \frac{b'^2 D_{KL} - v}{v e} \right) + 1. \tag{10}
\]

\[
s = \frac{1}{b'} \left( W \left( \frac{b'^2 D_{KL} - v}{v e} \right) + 1 \right). \tag{11}
\]
We note that Eq (10) is a consequence of the fact that the inverse function of \( y = xe^x \) is denoted by the Lambert \( W \) function. Since \( s > 0 \), we determine that \( W \) is the principal branch of the Lambert \( W \) function:

\[
    s = \frac{1}{b'} \left( W_0 \left( \frac{b'^2 D_{KL} - v}{ve} \right) + 1 \right). \tag{12}
\]

Substituting Eq. (12) into Eq. (7) and defining \( u := (b'^2 D_{KL} - v)/ve \) give the following result:

\[
    \mathcal{R}(q(\theta|S), q(\theta'|S')) \leq \frac{b'}{W_0(u) + 1} D_{KL} + \frac{v}{b'(W_0(u) + 1)} \phi(W_0(u) + 1) \tag{13}
\]

\[
= \frac{b'^2 D_{KL} - v}{b'(W_0(u) + 1)} + \frac{v}{b'(W_0(u) + 1)} \left( e^{W_0(u) + 1} - (W_0(u) + 1) - 1 \right) \tag{14}
\]

\[
= \frac{v}{b'(W_0(u) + 1)} \left( eu + e^{W_0(u) + 1} \right) - \frac{v}{b} \tag{15}
\]

\[
= \frac{v}{b'} \left( W_0(u)e^{W_0(u) + 1} + e^{W_0(u) + 1} \right) - \frac{v}{b} \tag{16}
\]

\[
= \frac{v}{b'} \left( e^{W_0(u) + 1} - 1 \right). \tag{17}
\]

In the above derivation, Eq. (15) is reduced to Eq. (16) by using the fact that \( (b'^2 D_{KL} - v) = veu \) because of the definition of \( u \), and Eq. (16) is reduced to Eq. (17) by using the fact that \( u = W_0(u)e^{W_0(u)} \). Suppose \( v = b'^2 \). Then, since \( u = (D_{KL} - 1)/e \), the following inequality holds:

\[
    \mathcal{R}(q(\theta|S), q(\theta'|S')) \leq b' \left\{ \exp \left( W_0 \left( \frac{D_{KL} - 1}{e} \right) + 1 \right) - 1 \right\}. \tag{19}
\]

The lower bound is proved by changing the sign in the proof for the upper bound, completing the proof of Theorem 1.

**Proof of Theorem 3** We assume \( \mathbb{E}[E_t|E_{t-1}^t] \leq E_{t-1} \), namely, \( E_{t-1}^t \) is assumed to be a supermartingale. We can apply the Doob–Meyer decomposition theorem to uniquely decompose \( E_t \) into martingale \( M_t \) and non-decreasing predictable process \( A_t \) as

\[
    E_t = M_t + A_t.
\]

Furthermore, \( M_t \) is written as

\[
    M_t = E_0 + \sum_{i=1}^{t} (E_i - \mathbb{E}[E_i|E_{i-1}^t])
\]

and

\[
    M_t - M_{t-1} = E_t - \mathbb{E}[E_t|E_{t-1}^t],
\]

where \( M_0 = E_0 \). From Theorem 1, we have

\[
    -(b-a)r(p(\theta|S_{t-1}), p(\theta|S_t)) - (A_t - A_{t-1}) \leq M_t - M_{t-1} \leq (b-a)r(p(\theta|S_t), p(\theta|S_{t-1})) - (A_t - A_{t-1}). \tag{20}
\]
By applying the Chernoff bound, the following inequality is derived:
\[
\Pr(M_t - M_{t-1} \geq \epsilon) \leq \min_{s > 0} e^{-s \mathbb{E}\left[e^{s(M_t - M_{t-1})}\right]}
\]
\[
\leq \min_{s > 0} e^{-s \mathbb{E}\left[e^{s(M_t - M_{t-1})|M_{t-1}}\right]}
\]
Since \(\mathbb{E}[M_t - M_{t-1}|M_{t-1}] = 0\), by applying Hoeffding’s lemma and Eq. (20), we have the following inequality:
\[
\mathbb{E}\left[e^{s(M_t - M_{t-1})|M_{t-1}}\right] \leq \exp\left(\frac{s^2(b - a)^2 r_t^2}{8}\right),
\]
where \(r_t = r(p(\theta|S_{t-1}), p(\theta|S_t)) + r(p(\theta|S_t), p(\theta|S_{t-1}))\). Thus,
\[
\Pr(M_t - M_{t-1} \geq \epsilon) \leq \min_{s > 0} \exp\left(\frac{s^2(b - a)^2 r_t^2}{8} - s \epsilon\right).
\]
Minimizing for \(s\) gives the upper bound
\[
\Pr(M_t - M_{t-1} \geq \epsilon) \leq \exp\left(-\frac{2 \epsilon^2}{(b - a)^2 r_t^2}\right).
\]
In the same way as above, we also have the following inequality:
\[
\Pr(M_t - M_{t-1} \leq -\epsilon) \leq \exp\left(-\frac{2 \epsilon^2}{(b - a)^2 r_t^2}\right),
\]
Combining the above inequalities, we have
\[
\Pr(|E_t - \mathbb{E}[E_t|E_{t-1}^t]| \leq \epsilon) \geq 1 - 2 \exp\left(-\frac{2 \epsilon^2}{(b - a)^2 r_t^2}\right).
\]
From the inequality, defining \(\delta = \{2 \exp(-2 \epsilon^2/(b - a)^2 r_t^2), \epsilon\}\), we have the following inequality with at least probability \(1 - \delta\):
\[
|E_t - \mathbb{E}[E_t|E_{t-1}^t]| \leq (b - a)\sqrt{-\frac{\log(\delta/2)}{2 r_t^2}}.
\]
We assume that right hand side of the inequality is smaller than \((b - a)\gamma\eta\):
\[
(b - a)\sqrt{-\frac{\log(\delta/2)}{2 r_t^2}} \leq (b - a)\gamma\eta.
\]
Then, we guarantee that \(|E_t - \mathbb{E}[E_t|E_{t-1}^t]|\) is smaller than \((b - a)\gamma\eta\) with at least probability \(1 - \delta\) when we stop active learning under the condition of Eq. (21).
Equation (21) leads to the following inequality:
\[
\lambda_t = \frac{r_t}{\gamma} \leq \sqrt{-\frac{2}{\log(\delta/2)}} \eta.
\]
Therefore, Theorem 3 is proved.
Appendix B. KL-divergence between GPs

Lemma 6 Let \( q(f|S) \) and \( q(f|S') \) be the posteriors with respect to \( \theta \) given \( S = (X,Y) \) and \( S' = (X',Y') \), respectively. We assume that the prior of \( q(f|S) \) is the same as that of \( q(f|S') \). Then, the following equation holds:

\[
D_{\text{KL}} [q(f|S)||q(f|S')] = D_{\text{KL}} [q(f_X|S)||q(f_X'|S')],
\]

where \( X_+ := X \cup X' \) and \( f_{X_+} := f(X_+) \).

Proof Let \( X_\Omega \) be a universal set of input data. We denote \( X_\Omega / X_+ \) by \( X_* \). From the chain rule of the KL-divergence (Gray, 2011), the following equation holds:

\[
D_{\text{KL}} [q(f|S)||q(f|S')]
= D_{\text{KL}} [q(f_X|S)||q(f_X'|S')]
+ \mathbb{E}_{q(f_X|S)} [D_{\text{KL}} [q(f_X|f_{X_+},S)||q(f_{X_*}|f_{X_+},S')]].
\]

(22)

We denote the prior of \( q(f_X|f_{X_+}|S) \) and \( q(f_{X_*}|f_{X_+}|S') \) by \( p(f_{X_*}, f_{X_+}) \). From the Bayesian theorem, the following equation holds:

\[
q(f_{X_*}|f_{X_+}, S) = \frac{p(f_{X_*}, f_{X_+}|S)}{p(f_{X_+}|S)}
= \frac{p(Y|f_{X_*}, X)p(f_{X_*}|f_{X_+})p(f_{X_+})}{p(Y|X)p(Y|f_{X_*}, X)p(f_{X_+})}
= \frac{p(f_{X_*}, f_{X_+})}{p(f_{X_+})} = p(f_{X_*}|f_{X_+}).
\]

Similarly, \( q(f_{X_*}|f_{X_+}, S') = p(f_{X_*}|f_{X_+}) \) also holds. Therefore, if the prior of \( q(f|S) \) is the same as that of \( q(f|S') \), the second term of Eq. (22) is zero. \( \blacksquare \)

Lemma 7 Let \( q(f|S_t) \) and \( q(f|S_{t-1}) \) be the GP posteriors given \( S_t = \{(x_i, y_i)\}_{i=1}^{n_t} \) and \( S_{t-1} = \{(x_i, y_i)\}_{i=1}^{n_{t-1}} \), respectively. We assume that the prior of \( q(f|S_t) \) is the same as that of \( q(f|S_{t-1}) \). Let \( \mu_t, \sigma_t \) and \( \beta \) be the mean and covariance functions of \( q(f|S_t) \) and the accuracy of Gaussian noise, respectively. Then, the following equation holds:

\[
D_{\text{KL}} [q(f|S_{t-1})||q(f|S_t)] = \frac{1}{2} \beta \sigma_{t-1}(x_{n_t}, x_{n_t}) - \frac{1}{2} \log (1 + \beta \sigma_{t-1}(x_{n_t}, x_{n_t}))
+ \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta - 1 (y_{n_t} - \mu_{t-1}(x_{n_t}))^2.
\]

Proof From Lemma 6, the following equation holds:

\[
D_{\text{KL}} [q(f|S_{t-1})||q(f|S_t)] = D_{\text{KL}} [q(f|S_{t-1})||q(f|S_t)],
\]

22
where $f := (f(x_1), f(x_2), \cdots, f(x_n))$. When $S_t = (X_t, Y_t)$ is observed, $q(f|S_t)$ can be described as

$$q(f|S_t) = \frac{p(Y_t|f, X_t)p(f)}{p(Y_t|X_t)}$$

$$= \frac{p(y_n|f, x_n)p(Y_{t-1}|f, X_{t-1})p(f)}{\int p(y_n|f', x_n)p(Y_{t-1}|f', X_{t-1})p(f')df'}$$

$$= \frac{\int p(y_n|f', x_n)p(Y_{t-1}|X_{t-1})q(f|S_{t-1})}{p(y_n|f, x_n)q(f|S_{t-1})}.$$ 

From this equation, $D_{KL}[q(f|S_{t-1})||q(f|S_t)]$ can be rewritten as

$$D_{KL}[q(f|S_{t-1})||q(f|S_t)]$$

$$= \mathbb{E}_{q(f|S_{t-1})} \left[ \log \frac{q(f|S_{t-1})p(y_n|f, x_n)}{p(y_n|f, x_n)q(f|S_{t-1})} \right]$$

$$= \log p(y_n|f, x_n) - \mathbb{E}_{q(f|S_{t-1})} \left[ \log p(y_n|f, x_n) \right]$$

$$= \log \int q(f_t|S_{t-1})p(y_n|f_t)df_t - \int q(f_t|S_{t-1}) \log p(y_n|f_t)df_t,$$  

(23)

where $f_t := f(x_{n_t})$. The first term of Eq. (23) becomes the logarithm of a normal distribution since $p(y_n|f_t)$ and $q(f_t|S_{t-1})$ are normal distributions. Specifically, from $p(y_n|f_t) = \mathcal{N}(y_n|f_t, \beta^{-1})$ and $p(f_t|S_{t-1}) = \mathcal{N}(f_t|\mu_{t-1}(x_n), \sigma_{t-1}(x_n, x_n))$, the following equation holds:

$$\log \int p(y_n|f_t)q(f_t|S_{t-1})df_t$$

$$= \log \mathcal{N}(y_n|\mu_{t-1}(x_n), \sigma_{t-1}(x_n, x_n) + \beta^{-1}).$$  

(24)

The second term can be rewritten as

$$- \int q(f_t|S_{t-1}) \log p(y_n|f_t)df_t = \mathbb{E}_{q(f_t|S_{t-1})} \left[ \frac{\beta}{2} (y_n - f_t)^2 \right] + \frac{1}{2} \log 2\pi \beta^{-1}$$

$$= \frac{\beta}{2} \left( y_n^2 - 2y_n \mathbb{E}[f_t] + \mathbb{E}[f_t^2] \right) + \frac{1}{2} \log 2\pi \beta^{-1}$$

$$= \frac{\beta}{2} (y_n - \mu_{t-1}(x_n))^2 + \frac{\beta}{2} \sigma_{t-1}(x_n, x_n) + \frac{1}{2} \log 2\pi \beta^{-1}.$$  

(25)
From the above equation, the lemma is derived as

\[
D_{KL} [q(f|S_t-1)||q(f|S_t)] \\
= -\frac{(y_{n_t} - \mu_{t-1}(x_{n_t}))^2}{2(\sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1})} - \frac{1}{2} \log 2\pi(\sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1}) \\
+ \frac{\beta}{2}(y_{n_t} - \mu_{t-1}(x_{n_t}))^2 + \frac{\beta}{2}\sigma_{t-1}(x_{n_t}, x_{n_t}) + \frac{1}{2} \log 2\pi\beta^{-1} \\
= \frac{1}{2}\beta\sigma_{t-1}(x_{n_t}, x_{n_t}) - \frac{1}{2} \log (1 + \beta\sigma_{t-1}(x_{n_t}, x_{n_t})) \\
+ \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1}(y_{n_t} - \mu_{t-1}(x_{n_t}))^2.
\]

Lemma 8 Let \( q(f|S_t) \) and \( q(f|S_{t-1}) \) be the GP posteriors given \( S_t = \{(x_i, y_i)\}_{i=1}^{n_t} \) and \( S_{t-1} = \{(x_i, y_i)\}_{i=1}^{n_{t-1}} \), respectively. We assume that the prior of \( q(f|S_t) \) is the same as that of \( q(f|S_{t-1}) \). Let \( \mu_t, \sigma_t \) and \( \beta \) be the mean and covariance functions of \( q(f|S_t) \), and the accuracy of Gaussian noise, respectively. Then, the following equation holds:

\[
D_{KL} [p(f|S_t)||p(f|S_{t-1})] = D_{KL} [p(f_{X_t}|S_t)||p(f_{X_t}|S_{t-1})] \\
= \frac{1}{2} \log (1 + \beta\sigma_{t-1}(x_{n_t}, x_{n_t})) - \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1} \\
+ \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t})(y_{n_t} - \mu_{t-1}(x_{n_t}))^2.
\]

Proof In analogy with Eq. (23), the following equation holds:

\[
D_{KL} [q(f|S_t)||q(f|S_{t-1})] \\
= \mathbb{E}_{q(f|S_t)} \left[ \log \frac{p(y_{n_t}|f, x_{n_t})q(f|S_{t-1})}{q(f|S_{t-1})p(y_{n_t}|x_{n_t})} \right] \\
= \mathbb{E}_{q(f|S_t)} \left[ \log p(y_{n_t}|f, x_{n_t}) \right] - \log p(y_{n_t}|x_{n_t}) \\
= \int q(f|S_t) \log p(y_{n_t}|f, x_{n_t}) df_t - \log \int q(f|S_{t-1})p(y_{n_t}|f_t, x_{n_t}) df_t,
\]

where \( f_t := f(x_{n_t}) \). The second term is the same as Eq. (24). In the same way as for Eq. (25), the first term is derived as

\[
\int q(f|S_t) \log p(y_{n_t}|f_t) df_t \\
= -\frac{\beta}{2}(y_{n_t} - \mu_t(x_{n_t}))^2 - \frac{\beta}{2}\sigma_t(x_{n_t}, x_{n_t}) - \frac{1}{2} \log 2\pi\beta^{-1}.
\]
Regarding \( q(f_t|S_t) \) as the posterior whose prior is \( q(f_t|S_{t-1}) \) observing \((x_{n_t}, y_{n_t})\), the values of the mean function and covariance function corresponding to \( x_{n_t} \) are derived as

\[
\begin{align*}
\mu_t(x_{n_t}) &= \mu_{t-1}(x_{n_t}) + \frac{\sigma_{t-1}(x_{n_t}, x_{n_t})}{\sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1}} (y_{n_t} - \mu_{t-1}(x_{n_t})) \\
&= \beta^{-1} \frac{\mu_{t-1}(x_{n_t}) + \sigma_{t-1}(x_{n_t}, x_{n_t}) y_{n_t}}{\sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1}} \\
\sigma_t(x_{n_t}, x_{n_t}) &= \sigma_{t-1}(x_{n_t}, x_{n_t}) - \frac{\sigma_{t-1}^2(x_{n_t}, x_{n_t})}{\sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1}} \\
&= \frac{\beta^{-1} \sigma_{t-1}(x_{n_t}, x_{n_t})}{\sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1}}.
\end{align*}
\]

From the result, the second term is rewritten as

\[
\int q(f_t|S_t) \log p(y_{n_t}|f_t) df_t = - \frac{1}{2} \beta^{-1} (y_{n_t} - \mu_{t-1}(x_{n_t}))^2 + \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t}) - \frac{1}{2} \log 2\pi \beta^{-1}.
\]

Therefore, the following equation holds:

\[
D_{KL}[q(f|S_t)||q(f|S_{t-1})] = \int q(f_t|S_t) \log p(y_{n_t}|f_t, x_{n_t}) df_t - \log \int q(f_t|S_{t-1}) p(y_{n_t}|f_t, x_{n_t}) df_t
\]

\[
= - \frac{1}{2} \beta^{-1} (y_{n_t} - \mu_{t-1}(x_{n_t}))^2 + \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t}) - \frac{1}{2} \log 2\pi \beta^{-1} + \frac{1}{2} \log 2\pi (\sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1})
\]

\[
= \frac{1}{2} \sigma_{t-1}(x_{n_t}, x_{n_t}) (y_{n_t} - \mu_{t-1}(x_{n_t}))^2 + \frac{1}{2} \log (1 + \beta \sigma_{t-1}(x_{n_t}, x_{n_t})) - \frac{1}{2} \frac{\sigma_{t-1}(x_{n_t}, x_{n_t})}{\sigma_{t-1}(x_{n_t}, x_{n_t}) + \beta^{-1}}.
\]

Appendix C. Tight bound for the KL-divergence between dropout-based deep Bayes posteriors

**Lemma 9** Let \( p(\theta) \) and \( q(\theta) \) be posterior distributions with respect to a dropout-based Bayesian deep neural network. Namely, the posterior distribution is assumed to have the following form:

\[
p(\theta) = \prod_{l=1}^{L} p(W_l)p(b_l),
\]

\[25\]
where

\[
p(W_l) = \prod_{h=1}^{H_l-1} p(w_{lh})
\]

\[
p(b_l) = \mathcal{N}(\nu_l, \sigma_l^2 I)
\]

and

\[
p(w_{lh}) = p_l \mathcal{N}(m_{lh}, \sigma_l^2 I) + (1 - p_l) \mathcal{N}(0, \sigma_l^2 I).
\]

Now, \(D_{KL}[p(\theta)||q(\theta)]\) is upper bounded as

\[
D_{KL}[p(\theta)||q(\theta)] \leq \frac{1}{2} \sum_{l=1}^{L} \left\{ \frac{p_l}{\sigma_l^2} \| M_l - M'_l \|^2 + \frac{1}{\sigma_l^2} \| \nu_l - \nu'_l \|^2 + H_{l-1} D_{KL}[p_l||q_l] \right\}
\]

\[
+ \sum_{l=1}^{L} \frac{(1 + p_l H_{l-1}) H_l}{2} \left\{ \frac{\sigma_l^2}{\sigma_l'^2} - \log \frac{\sigma_l^2}{\sigma_l'^2} - 1 \right\},
\]

where \(M_l := (m_{l1}, m_{l2}, \ldots, m_{lH_l})\) and \(D_{KL}[p_l||q_l] := p_l \log \frac{p_l}{q_l} + (1 - p_l) \log \frac{1 - p_l}{1 - q_l} \).

**Proof** From \(p(\theta) = \prod_{l=1}^{L} p(W_l) p(b_l)\), we obtain

\[
D_{KL}[p(\theta)||q(\theta)] = \int \prod_{l=1}^{L} p(W_l) p(b_l) \log \frac{\prod_{l=1}^{L} p(W_l) p(b_l)}{\prod_{l=1}^{L} q(W_l) q(b_l)} dW_l db_l
\]

\[
= \sum_{l=1}^{L} \int p(W_l) p(b_l) \log \frac{p(W_l) p(b_l)}{q(W_l) q(b_l)} dW_l db_l
\]

\[
= \sum_{l=1}^{L} \int p(W_l) \log \frac{p(W_l)}{q(W_l)} dW_l + \sum_{l=1}^{L} \int p(b_l) \log \frac{p(b_l)}{q(b_l)} db_l
\]

\[
= \sum_{l=1}^{L} \sum_{h=1}^{H_{l-1}} D_{KL}[p(w_{lh})||q(w_{lh})] + \sum_{l=1}^{L} D_{KL}[p(b_l)||q(b_l)].
\]

The second term of the above formula is the summation of the KL-divergences between Gaussians and has an analytical expression, though the first term is the summation of the KL-divergences between mixture distributions and does not have an analytical solution. We consider the upper bound of the first term by introducing a latent variable \(z_{lh} \in \{0, 1\}\) into \(p(w_{lh})\) to indicate the correspondence between the mixture and \(w_{lh}\). The chain rule of the KL-divergence leads to

\[
D_{KL}[p(w_{lh}, z_{lh})||q(w_{lh}, z_{lh})] \geq D_{KL}[p(w_{lh})||q(w_{lh})].
\]

Since we do not know the correspondence between latent variables of GMMs, the joint distribution \(p(w_{lh}, z_{lh})\) is written as

\[
p(w_{lh}, z_{lh}) = p(w_{lh}|z_{lh}) p(z_{lh}) = p_{z_{lh}} \mathcal{N}(z_{lh} m_{lh}, \sigma_l^2 I),
\]
while the joint distribution \( q(w_{lh}, z_{lh}) \) is written as
\[
q(w_{lh}, z_{lh}) = q_{\pi(z_{lh})}N(\pi(z_{lh})m_{lh}, \sigma_l^2 I),
\]
where \( \pi(z) \) is any permutation. Then, the KL-divergence between these joint distributions is analytically computable as
\[
DL[p(w_{lh}, z_{lh})||q(w_{lh}, z_{lh})] = \int \sum_{z \in \{0, 1\}} p(w_{lh}, z_{lh} = z) \log \frac{p(w_{lh}, z_{lh} = z)}{q(w_{lh}, z_{lh} = z)} dw_{lh}
\]
\[
= \sum_{z \in \{0, 1\}} DL[p(w_{lh}, z_{lh} = z)||q(w_{lh}, z_{lh} = z)]
\]
\[
= \sum_{z \in \{0, 1\}} pz \left[ DL[N(zm_{lh}, \sigma_l^2 I)||N(\pi(z)m_{lh}', \sigma_l^2 I)] + \log \frac{pz}{q_{\pi(z)}} \right].
\]

Equation (27) holds for any \( \pi(z) \), but it is preferable to set the latent variable with a tighter bound. In our case, there are two mixture components and it is also known that the centroid of one of those two components must be zero and that the two components share the same variance. In this situation, by setting \( \pi(z) = z \), we can minimize the KL-divergence between joint distributions. Now we have the following tighter upper bound:
\[
DL[p(w_{lh})||q(w_{lh})] = \sum_{l=1}^{L} DL[p_{lh}[\mu_l, \sigma_l^2 ]||q_{lh}[\mu_l, \sigma_l^2 ]] + DL[p_{lh}||q_{lh}]
\]
\[
= \frac{1}{2} \sum_{l=1}^{L} \left( H_l \frac{\sigma_l^2}{\sigma_l^2} - H_l \log \frac{\sigma_l^2}{\sigma_l^2} + \frac{1}{\sigma_l^2} \| \mu_l - \mu_l' \|^2 - H_l + DL[p_{lh}||q_{lh}] \right)
\]
\[
\geq DL[p(w_{lh})||q(w_{lh})].
\]

Substituting the result into Eq. (26) leads to the following inequality:
\[
DL[p(\theta)||q(\theta)] 
\]
\[
\leq \sum_{l=1}^{L} \sum_{h=1}^{H_l} \frac{p_l}{2} \left\{ H_l \frac{\sigma_l^2}{\sigma_l^2} - H_l \log \frac{\sigma_l^2}{\sigma_l^2} + \frac{1}{\sigma_l^2} \| \mu_l - \mu_l' \|^2 - H_l + DL[p_{lh}||q_{lh}] \right\}
\]
\[
+ \frac{1}{2} \sum_{l=1}^{L} \left\{ H_l \frac{\sigma_l^2}{\sigma_l^2} - H_l \log \frac{\sigma_l^2}{\sigma_l^2} + \frac{1}{\sigma_l^2} \| \nu_l - \nu_l' \|^2 - H_l \right\}
\]
\[
= \frac{1}{2} \sum_{l=1}^{L} \left\{ \frac{p_l}{\sigma_l^2} \| M_l - M_l' \|^2 + \frac{1}{\sigma_l^2} \| \nu_l - \nu_l' \|^2 + H_l - DL[p_{lh}||q_{lh}] \right\}
\]
\[
+ \sum_{l=1}^{L} \frac{1 + p_l H_{l-1}}{2} H_l \left\{ \frac{\sigma_l^2}{\sigma_l^2} - \log \frac{\sigma_l^2}{\sigma_l^2} - 1 \right\}. \]
\]
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