Characterizing the robustness of Bayesian adaptive experimental designs to active learning bias

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Abstract

Bayesian adaptive experimental design is a form of active learning, which chooses samples to maximize the information they give about uncertain parameters. Prior work has shown that other forms of active learning can suffer from active learning bias, where unrepresentative sampling leads to inconsistent parameter estimates. We show that active learning bias can also afflict Bayesian adaptive experimental design, depending on model misspecification. We develop an information-theoretic measure of misspecification, and show that worse misspecification implies more severe active learning bias. We also show that model classes incorporating more “noise” — i.e., specifying higher inherent variance in observations — suffer less from active learning bias, because their predictive distributions are likely to overlap more with the true distribution.

Keywords: active learning, optimal experimental design, Bayesian inference, mathematical modeling, model misspecification

Adaptive sampling methods choose data points in sequence to be as informative as possible (Cavagnaro et al., 2010; Ryan et al., 2016). In machine learning, this is called active learning (Kanamori, 2002; Settles, 2012). Despite their advantages, adaptive sampling schemes can produce training sets that are highly unrepresentative of the target distribution.

1. We will use “adaptive sampling” and “active learning” interchangeably.
(Farquhar et al., 2021), and the estimates made from adaptively-sampled data may not generalize to the target. This phenomenon is **active learning bias** (Farquhar et al., 2021).

We study the presence of active learning bias in a class of active learning methods called information theoretic active learning, where the modeler must pick an objective function capturing the informativeness of observations (Houlsby et al. 2011). These methods have been studied in parallel fields, such as computerized adaptive testing (Owen 1969), clinical research (Whitehead and Brunier, 1995) and cognitive modeling (Cavagnaro et al., 2010), where they are referred to as **Bayesian sequential (or adaptive) experimental design** (Drovandi et al. 2013 Ryan et al., 2016) or adaptive design optimization (Cavagnaro et al., 2010).

### 1. Active learning bias and model misspecification

The advantages of active learning methods are usually expounded assuming that the model class is well-specified, i.e., that the true data-generating distribution is a member of the class (MacKay, 1992; Kanamori, 2002; Dasgupta, 2004; Sugiyama, 2005; Myung et al., 2013). Yet in most modeling enterprises, this assumption is not credible: the exact form of the true data-generating process is difficult if not impossible to know, and models are deliberately simplified tractable approximations.

While sampling bias and vulnerability to model misspecification are often discussed as two separate limitations of active learning methods, it turns out they are deeply related. In particular, sampling bias, or covariate shift, can amplify bias when the model class is misspecified (Sugiyama et al., 2008; Wen et al., 2014; Spencer et al., 2021). The implication of this is that active learning methods can increase bias when the model class is misspecified (Sugiyama, 2005; Bach, 2006).

### 2. Contributions of the present work

We apply insights on active learning bias from the machine learning literature to Bayesian adaptive experimental designs, and investigate how the extent of active learning bias varies with degree of model misspecification. We also demonstrate how the amount of observational “noise” specified by a model can mitigate active learning bias, since the former affects the model’s degree of misspecification.

### 3. Preliminaries and notation

A modeler wants to predict some variable $y \in \mathbb{R}^m$ using another variable $x \in \mathbb{R}^d$. Given $x$, $y$ always follows the same distribution, $y|x \sim f(x)$. We call $f$ the **true model**. We assume that $x$ is fully observable and follows some distribution $g$.

The modeler specifies a **hypothesized model class** that predicts $y|x \sim m(x, \theta)$, with $\theta \in \Theta$; the variable $\theta$ contains the **parameters** of the model class, which live in the **parameter space** $\Theta$. $\Theta$ is fixed, i.e. determined in advance of the data and unchanging in response to them. $m$ is a probabilistic function, whose form is also presumed to be fixed (e.g., logistic regression). The hypothesized model class $m(x, \Theta)$ is thus comprised of the set of distributions $\{m(x, \theta) : \theta \in \Theta\}$.
The model estimation problem is to find $\theta^* \in \Theta$ which minimizes the risk, i.e., such that

$$\theta^* \equiv \arg\min_{\theta \in \Theta} E \left[ \mathcal{L}(m(x, \theta), y) \right]$$ (1)

for some suitable loss function $\mathcal{L}$, which takes as inputs a predictive distribution and a realized value for $y$. Here, the expectation is under the true data-generating distribution, i.e., the product of $g$ and $f$. $m(x, \theta^*)$ is an instance of the hypothesized model class, the best-fitting model.

To estimate $\theta^*$, the modeler gets a set of samples $x \in \mathbb{R}^{n \times d}$ and observes outcomes $y \in \mathbb{R}^{n \times m}$. We consider only distributional estimates of $\theta^*$, essentially assigning a probability to each $\theta \in \Theta$ that it is the risk minimizer:

$$p(\theta) \equiv P(\theta = \theta^* | x, y)$$ (2)

We refer to the corresponding predictive distribution for $y|x$ as $m(x, \hat{\theta})$. We call $m(x, \hat{\theta})$ the trained or estimated model.

Random sampling or passive learning techniques draw $x$ values IIDly from the population distribution $g$. Adaptive sampling or active learning techniques actively construct $x$ to maximize the concentration of $p$. Both then get $y|x \sim f(x)$. We write $m(x, \hat{\theta}_{\text{adaptive}})$ for the result of an adaptive procedure, and $m(x, \hat{\theta})$, unmodified, for passive learning.

Note that risk, the modeler’s objective, is defined using the distribution $g$, the target distribution of inputs whose consequences the modeler ultimately wants to predict. Active learning bias (ALB) occurs when, averaging over data sets $x \sim g$ and corresponding observations $y|x \sim f$, $E \left[ \mathcal{L}(m(x, \hat{\theta}_{\text{adaptive}}), y) \right] > E \left[ \mathcal{L}(m(x, \theta^*), y) \right]$.

Finally, we say that a hypothesized model class is misspecified when the true model is not in the class, i.e., $f(x) \neq m(x, \theta)$ for all $\theta \in \Theta$. Consistent with prior literature, we say “model misspecification,” even though it is the hypothesized model class that is wrong.

### 4. Bayesian adaptive experimental design

A natural way to construct $p$ is via Bayesian inference. We begin with a prior distribution $p_0$, and, at the $t^{th}$ step, where we observe $x_t$ and $y_t$, we use Bayes’s rule to update it recursively

$$p_t(\theta) = p_{t-1}(\theta) \frac{m(y_t|x_t, \theta)}{\int_\theta m(y_t|x_t, \theta) p_{t-1}(\theta) d\theta}$$ (3)

Here, $m(y_t|x_t, \theta)$ indicates the likelihood of observation $y_t$ under the distribution $m(x_t, \theta)$.

$p_t(\theta)$ thus implicitly involves the whole history of inputs and responses to date, $x_t$ and $y_t$ respectively.

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2. Related work writes of selecting a hypothesis from a hypothesis class (Dasgupta, 2004; Golovin et al., 2010). Our “hypothesized model class” matches their “hypothesis class,” and selecting $\theta^*$ from $\Theta$ amounts to selecting a hypothesis from the hypothesis class. Our terminology is similar to Shiffrin and Chandramouli (2016), who also distinguish between model classes and model instances in the context of Bayesian modeling.

3. We use this notation for brevity, but note that there need not be a single $\theta \in \Theta$ giving exactly this distribution.
For Bayesian adaptive designs, at every step \( t \) we define the modeler’s expected utility of an input \( x \) over the current posterior distribution of \( \theta \):

\[
E[u_t(x)] = \int_{\theta} \int_{y} u(x, y, \theta) \ m(y|x, \theta) \ p_{t-1}(\theta) \ dy \ d\theta
\]  

Bayesian adaptive experimental designs pick the maximizer of \( E[u_t(x)] \) as the next value of \( x \). We pick a \( u \) that encourages precision of parameter estimates:

\[
u(x, y, \theta) = \log \frac{p_{t-1}(\theta|y, x)}{p_{t-1}(\theta)}
\]

5. Results

We here compare the behavior of Bayesian adaptive experimental designs in the case of a misspecified vs. well-specified class of polynomial regression models. In the extended version of this paper (Sloman et al., 2022), we show that our findings apply to both a toy classification problem and a preference-learning problem.

Figures 1a–1c show the results of several simulations in which \( f \) is a degree-two polynomial regression model, i.e., \( y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon \) where \( \epsilon \sim \mathcal{N}(0, 100) \). In the underparameterized case (Figure 1a), \( m \), the functional form corresponding to the hypothesized model class, is linear in \( x \). In the fully parameterized case (Figure 1b), \( m \) is quadratic in \( x \). In the overparameterized case (Figure 1c), \( m \) is cubic. In all cases, the additive noise is (correctly) specified as \( \epsilon \sim \mathcal{N}(0, 100) \). Thus, by our definition, only the underparameterized case is misspecified.

Behavior in the misspecified (underparameterized) case is markedly different from the behavior in the other two cases. Risk was measured as the negative log likelihood (NLL) of 100 observations drawn randomly from the target distribution, \( g = \text{Unif}(0, 100) \). For the well-specified model classes, adaptive sampling reduces the risk more quickly than random sampling, though both converge on the same risk as \( \theta^* \). However, under misspecification, Bayesian adaptive designs lead to worse generalization than random sampling.

5.1 ALB depends on degree of misspecification

We now investigate how the extent of ALB varies with the degree of misspecification. There is a natural information-theoretic way to measure the latter, using the Kullback-Leibler divergence (KLD). Concretely, we define the degree of misspecification as the expectation, under \( g \), of the KLD between the true \( f \) and the best-fitting model:

\[
\mathcal{D}_{\text{model}} = \int_{x} \text{KLD}(f(x), m(x, \theta^*)) \ g(x) \ dx
\]

4. With this choice of \( u \), \( E[u_t] \) is the mutual information between the next observation and the parameter \( \theta \), regarded as a random variable distributed according to \( p \) (Bernardo 1979; Myung et al., 2013; Ryan et al., 2016).

5. When using adaptive sampling, we identified the optimal design at each time step \( t \) using the \texttt{iminuit} package (Dembinski et al., 2020) and numerically integrating the expected utility function shown in equation 4 for 4,000 samples from the parameter distribution at \( t-1 \).

6. We found \( \theta^* \) by taking the OLS solution to a regression of 1,001 evenly spaced points across the domain and their expectation under the true model.
(a) $m$ is linear, with additive noise $\epsilon \sim \mathcal{N}(0, 100)$.

(b) $m$ is quadratic, with additive noise $\epsilon \sim \mathcal{N}(0, 100)$.

(c) $m$ is cubic, with additive noise $\epsilon \sim \mathcal{N}(0, 100)$.

(d) $m$ is linear, with additive noise $\epsilon \sim \mathcal{N}(0, 1000)$.

Figure 1: Risk incurred across 100 steps of Bayesian updating. Risk is approximated as the negative log likelihood (NLL) of 100 observations from the target distribution. The generating model is always a degree-two polynomial with parameters drawn from a $\mathcal{N}([0, 0, 0], \text{diag}(100, 10, .1))$ distribution. Lines are means across 1,000 simulated experiments, with error bars showing $\pm 1$ standard error around the mean. Horizontal lines show the risk achievable by $m(x, \theta^*)$. Green lines (---) show results using Bayesian adaptive design optimization during model estimation. Orange lines (--) show results using random sampling from the target distribution.

We define ALB as

$$ ALB \equiv \frac{\mathbf{E} [\mathcal{L}(m(x, \hat{\theta}_{\text{adaptive}}), y)]}{\mathbf{E} [\mathcal{L}(m(x, \theta^*), y)]} - 1 $$

(7)

$ALB$ is thus proportion of expected risk in excess of what the best parameter value would deliver.

We analyzed the $ALB$ values from the simulated experiments shown in Figure 1a as a function of the corresponding $\mathcal{P}_{\text{model}}$ values. (To calculate $ALB$, we approximated the risk by the $\text{NLL}$ of 100 observations from the target distribution. $\mathbf{E} [\mathcal{L}(m(x, \hat{\theta}_{\text{adaptive}}), y)]$ was calculated as the $\text{NLL}$ assigned by the estimated model after 100 steps of Bayesian adaptive design optimization — the same values shown as the rightmost point of the green
We found a very strong correlation between the two of .95 ($p = .00$). In other words, more misspecification predicted more ALB.

One way to adjust $D_{\text{model}}$ is by specifying a “noisier” model class, i.e., to force $m$ to predict more inherent variation in its outputs. As the predictive distribution corresponding to the hypothesized model class becomes more dispersed, it will overlap more with the data-generating distribution, leading to a lower divergence from $f$ to the hypothesized model class, and thus to lower misspecification. This suggests that if the degree of ALB depends on $D_{\text{model}}$, then ALB should be reduced, or even eliminated, by specifying noisier models.

Figure 1d shows the evolution of risk for the misspecified model class of the form shown in Figure 1a. However, instead of additive noise distributed $\mathcal{N}(0,100)$, the hypothesized model class incorporates additive noise distributed $\mathcal{N}(0,1000)$. Figure 1d shows that the incorporation of this additional noise nearly eliminates the ALB, which is reminiscent of theoretical results in Sugiyama (2005) that active learning is robust to model classes that are only slightly misspecified.$^7$

6. Discussion

We demonstrated that active learning bias can afflict Bayesian adaptive experimental designs, that the extent of active learning bias varies with the degree of model misspecification, and that the amount of observational noise specified by the model class mitigates the extent of active learning bias. Subsequent work should investigate the existence of mathematical bounds on the amount of noise needed for a model class to be tolerant to active learning bias,$^8$ as well as the applicability of our findings in more realistic modeling scenarios.

Author note

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7. We also found the same qualitative relationship between degree of misspecification, ALB and anticipated observational noise for a model misspecified as quadratic in $x$ when the generating model was cubic. These results are reported in the extended version of this paper (Sloman et al., 2022).

8. Such a study could perhaps draw from theoretical results on the tolerance of parameterized bandit learning algorithms to misspecification (Kannan et al. 2018. Bogunovic and Krause. 2021).
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