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A Method for Avoiding Bias from Feature Selection with Application to Naive Bayes Classification Models

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Abstract. For many classification and regression problems, a large number of features are available for possible use — this is typical of DNA microarray data on gene expression, for example. Often, for computational or other reasons, only a small subset of these features are selected for use in a model, based on some simple measure such as correlation with the response variable. This procedure may introduce an optimistic bias, however, in which the response variable appears to be more predictable than it actually is, because the high correlation of the selected features with the response may be partly or wholely due to chance. We show how this bias can be avoided when using a Bayesian model for the joint distribution of features and response. The crucial insight is that even if we forget the exact values of the unselected features, we should retain, and condition on, the knowledge that their correlation with the response was too small for them to be selected. In this paper we describe how this idea can be implemented for "naive Bayes" models of binary data. Experiments with simulated data confirm that this method avoids bias due to feature selection. We also apply the naive Bayes model to subsets of data relating gene expression to colon cancer, and find that correcting for bias from feature selection does improve predictive performance.

1 Introduction

Regression and classification problems that have a large number of available "features" (also known as "inputs", "covariates", or "predictor variables") are becoming increasingly common. Such problems arise in many application areas. Data on the expression levels of tens of thousands of genes can now be obtained using DNA microarrays, and used for tasks such as classifying tumors. Document analysis may be based on counts of how often each word in a large dictionary occurs in each document. Commercial databases may contain hundreds of features describing each customer.

Using all the features available in such problems is often infeasible. Using too many features can result in "overfitting" when simple statistical methods such as maximum likelihood are used, with the consequence that poor predictions are made for the response variable (e.g., the class) in new items. More sophisticated Bayesian methods can avoid such statistical problems, but using a large number of features may still be undesirable. We will focus primarily on situations where the computational cost of looking at all features is too burdensome. Another issue in some applications is that using a model that looks at all features will require measuring all these features when making predictions for future items, which may sometimes be costly. In some situations, models using few features may be preferred because they are easier to interpret.

For such reasons, modelers often use only a subset of features, chosen by some simple indicator of how useful they might be in predicting the response variable — see, for example, the papers in (Guyon, *et al.* 2006). For both regression problems with a real-valued response variable and classification problems with a binary (0/1) class variable, one suitable measure of how useful a feature may be is the sample correlation of the feature with the response. If the absolute value of this sample correlation is small, we might decide to omit the feature from our model. This criterion is not perfect, of course — it may result in a relevant feature being ignored if its relationship with the response is non-linear, and it may result in many redundant features being retained even when they all contain essentially the same information. Sample correlation is easily computed, however, and hence is an attractive criterion for screening a large number of features.

Unfortunately, a model that uses only a subset of features, selected based on their high correlation with the response, will be optimistically biased — i.e., predictions made using the model will (on average) be more confident than is actually warranted. For example, we might find that the model predicts that certain items belong to class 1 with probability 90%, when in fact only 70% of these items are in class 1. In a situation where the class is actually completely unpredictable from the features, a model using a subset of features that purely by chance had high sample correlation with the class may produce highly confidence predictions that have less actual chance of being correct than just guessing the most common class.

This optimistic bias comes from ignoring a basic principle of Bayesian inference — that we should base our conclusions on probabilities that are conditional on *all* the available information. If we have an appropriate model, this principle would lead us to use all the features. This would produce the best possible predictive performance. However, we assume here that computational or other pragmatic issues make using all features unattractive. When we therefore choose to "forget" some features, we can nevertheless still retain the information about how we selected the subset of features that we use in the model. Properly conditioning on this information when forming the posterior distribution eliminates the bias from feature selection, producing predictions that are as good as possible given the information in the selected features, without the overconfidence that comes from ignoring the feature selection process.

In the next section, we describe this idea in more detail, and discuss the difficulties of implementing it. We then show how the idea can be applied to a simple "naive Bayes" classification model with binary features that are assumed to be independent given the value of the response variable. We apply this naive Bayes model to simulated data and to data regarding gene expression in colon cancer, showing that bias correction does indeed improve predictions. Our method is more generally applicable, however. In the final section, we briefly discuss our work on mixture models for binary data and on factor analysis models for real-valued data, as well as other possible applications.

2 Our method for avoiding selection bias

Suppose we wish to predict a response variable, y, based on the information in the numerical features $x_1, \ldots, x_p$, which we sometimes write as a vector, $\boldsymbol{x}$. Our method is applicable both when y is a binary (0/1) class indicator, as is the case for the naive Bayes models discussed later, and when y is real-valued. We assume that we have complete data on n "training" cases, for which the responses are $y^{(1)}, \ldots, y^{(n)}$ (collectively written as y^{train}) and the feature vectors are $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)}$ (collectively written as $\boldsymbol{x}^{\text{train}}$). (Note that when y, $\boldsymbol{x}$, or x_t are used without a superscript, they will refer to some unspecified case.) We wish to predict the response for one or more "test" cases, for which we know only the feature vector. Our predictions will take the form of a distribution for y, rather than just a single-valued guess.

We are interested in problems where the number of features, p, is quite big — perhaps as large as ten or a hundred thousand — and accordingly (for pragmatic reasons) we intend to select a subset of features based on the absolute value of each feature's sample correlation with the response. The sample correlation of the response with feature t is defined as follows (or as zero if the denominator below is zero):

$$\text{COR}(y^{\text{train}}, x_t^{\text{train}}) \;=\; \frac{\displaystyle\sum_{i=1}^{n} \left(y^{(i)} - \bar{y}\right)\left(x_t^{(i)} - \bar{x}_t\right)}{\sqrt{\displaystyle\sum_{i=1}^{n} \left(y^{(i)} - \bar{y}\right)^2}\;\sqrt{\displaystyle\sum_{i=1}^{n} \left(x_t^{(i)} - \bar{x}_t\right)^2}} \tag{1}$$

where $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y^{(i)}$ and $\bar{x}_t = \frac{1}{n}\sum_{i=1}^{n} x_t^{(i)}$. The numerator can be simplified to $\sum_{i=1}^{n} \left(y^{(i)} - \bar{y}\right)x_t^{(i)}$.

Although our interest is only in predicting the response, we assume that we have a model for the joint distribution of the response together with all the features. From such a joint distribution, with probability or density function $P(y, x_1, \ldots, x_p)$, we can obtain the conditional distribution for y given any subset of features, for instance $P(y \,|\, x_1, \ldots, x_k)$, with $k < p$. This is the distribution we need in order to make predictions based on this subset. Note that selecting a subset of features makes sense only when the omitted features can be regarded as random, with some well-defined distribution given the features that are retained, since such a distribution is essential for these predictions be meaningful. This can be seen from the following expression:

$$\begin{aligned} &P(y \,|\, x_1, \ldots, x_k) \\ &\quad = \int \cdots \int P(y \,|\, x_1, \ldots, x_k, x_{k+1}, \ldots, x_p)\; P(x_{k+1}, \ldots, x_p \,|\, x_1, \ldots, x_k)\; dx_{k+1} \cdots dx_p \end{aligned} \tag{2}$$

If $P(x_{k+1}, \ldots, x_p \,|\, x_1, \ldots, x_k)$ does not exist in any meaningful sense — as would be the case, for example, if the data were collected by an experimenter who just decided arbitrarily what to set $x_{k+1}, \ldots, x_p$ to — then $P(y \,|\, x_1, \ldots, x_k)$ will also have no meaning.

Consequently, features that cannot usefully be regarded as random should always be retained. Our general method can accommodate such features, provided we use a model for the joint distribution of the response together with the random features, conditional on given values for the non-random features. However, for simplicity, we will ignore the possible presence of non-random features in this paper.

We will assume that a subset of features is selected by fixing a threshold, γ, for the absolute value of the correlation of a selected feature with the response. We then omit feature t from the feature subset if $|\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \leq \gamma$, retaining those features with a greater degree of correlation. Another possible procedure is to fix the number of features, k, that we wish to retain, and then choose the k features whose correlation with the response is greatest in absolute value, breaking any tie at random. If s is the retained feature with the weakest correlation with the response, we can set γ to $|\text{COR}(y^{\text{train}}, x_s^{\text{train}})|$, and we will again know that if t is any omitted feature, $|\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \leq \gamma$. If either the response or the features have continuous distributions, exact equality of sample correlations will have probability zero, and consequently this situation can be treated as equivalent to one in which we fixed γ rather than k. If sample correlations for different features can be exactly equal, we should theoretically make use of the information that any possible tie was broken the way that it was, but ignoring this subtlety is unlikely to have any practical effect, since ties are still likely to be rare.

Regardless of the exact procedure used to select features, we will denote the number of features retained by k, we will renumber the features so that the subset of retained features is $x_1, \ldots, x_k$, and we will assume we know that $|\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \leq \gamma$ for $t = k+1, \ldots, p$.

We can now state the basic principle behind our bias-avoidance method: When forming the posterior distribution for parameters of the model using a subset of features, we should condition not only on the values in the training set of the response and of the k features we retained, but also on the fact that the other $p-k$ features have sample correlation with the response that is less than γ in absolute value. That is, the posterior distribution should be conditional on the following information:

$$y^{\text{train}}, \quad \boldsymbol{x}_{1:k}^{\text{train}}, \quad |\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \leq \gamma \text{ for } t = k+1, \ldots, p \tag{3}$$

where $\boldsymbol{x}_{1:k}^{\text{train}} = (x_1^{\text{train}}, \ldots, x_k^{\text{train}})$.

We claim that this procedure of conditioning on the fact that selection occurred will eliminate the bias from feature selection. Here, "bias" does not refer to estimates for model parameters, but rather to our estimate of how well we can predict responses in test cases. Bias in this respect is also referred to as a lack of "calibration" — that is, the predictive probabilities do not represent the actual chances of events (Dawid 1982). If the model describes the actual data generation mechanism, and the actual values of the model parameters are indeed randomly chosen according to our prior, Bayesian inference always produces well-calibrated results, on average (with respect to the distribution of data and parameter values chosen from the prior).

In justifying our claim that this procedure avoids selection bias, we will assume that our model for the joint distribution of the response and all features, and the prior we chose for it, are appropriate for the problem, and that we would therefore not see bias if we predicted the response using all the features. Now, imagine that rather than selecting a subset of features ourselves, after seeing all the data, we instead set up an automatic mechanism to do so, providing it with the value of γ to use as a threshold. This mechanism, which has access to all the data, will compute the sample correlations of all the features with the response, select the subset of features by comparing these sample correlations with γ, and then erase the values of the omitted features, delivering to us only the identities of the selected features and their values in the training cases. If we now condition on all the information that *we* know, but not on the information that was available to the selection mechanism but not to us, we will obtain unbiased inferences. The information we know is just that of (3) above.

Our method requires computation of an adjustment factor, $P(\mathcal{S} \mid \alpha,\, y^{\text{train}})$, where α is the set of parameters whose likelihood needs adjusting, and $\mathcal{S}$ represents the information regarding selection, namely that $|\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \,\leq\, \gamma$ for $t = k+1, \ldots, p$. Computing this factor is much easier if the x_t^{train} are conditionally independent given α and y^{train}, since we can then write it as a product of factors pertaining to the various omitted features. For the models we consider, these factors are also *all the same*, since nothing distinguishes one omitted feature from another. We can then write

$$
\begin{aligned}
P(\mathcal{S} \mid \alpha,\, y^{\text{train}}) \;&=\; \prod_{t=k+1}^{p} P\big(|\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \,\leq\, \gamma \mid \alpha,\, y^{\text{train}}\big) \qquad (4)\\
&=\; \Big[P\big(|\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \,\leq\, \gamma \mid \alpha,\, y^{\text{train}}\big)\Big]^{p-k} \qquad (5)
\end{aligned}
$$

where in the second expression, t represents *any* of the omitted features. Note that in this expression, y^{train} is conditioned on, and hence considered fixed, whereas x_t^{train} is random. Since the time needed to compute this adjustment factor does not depend on the number of omitted features, we may hope to save a large amount of computation time by omitting many features.

Computing the single factor we do need is not trivial, however, since it involves integrals over both x_t^{train} and any parameters specific to particular features. As we will see, however, efficient computation is possible for the naive Bayes model.

3 Application to naive Bayes models with binary features

In this section we show how to apply the bias correction method to Bayesian naive Bayes models in which both the features and the response are binary. Binary features are natural for some problems (e.g., test answers that are either correct or incorrect), or may result from thresholding real-valued features. Such thresholding can sometimes be beneficial — in a document classification problem, for example, whether or not a word is used at all may be more relevant to the class of the document than how many times it is used. Naive Bayes models assume that features are independent given the response. This assumption is often incorrect, but such simple naive Bayes models have nevertheless been found to work well for many practical problems. Here we show how to correct for selection bias in binary naive Bayes models, whose simplicity allows the required adjustment factor to be computed very quickly. Simulations reported in the next section show that substantial bias can be present with the uncorrected method, and that it is indeed corrected by conditioning on the fact that feature selection occurred. We then apply the method to real data on gene expression relating to colon cancer, and again find that our bias correction method improves predictions.

3.1 Definition of the binary naive Bayes model

Let $\boldsymbol{x}^{(i)} = (x_1^{(i)}, \cdots, x_p^{(i)})$ be the vector of p binary features for case i, and let $y^{(i)}$ be the binary response for case i, indicating the class. For example, $y^{(i)} = 1$ might indicates that cancer is present for patient i, and $y^{(i)} = 0$ indicate that cancer is not present. Cases are assumed to be independent given the values of the model parameters (ie, exchangeable *a priori*). The probability that $y = 1$ in a case is given by the parameter ψ. Conditional on the class y in some case (and on the model parameters), the features $x_1, \ldots, x_p$ are assumed to be independent, and to have Bernoulli distributions with parameters $\phi_{y,1}, \ldots, \phi_{y,p}$, collectively written as $\boldsymbol{\phi}_y$, with $\boldsymbol{\phi} = (\boldsymbol{\phi}_0, \boldsymbol{\phi}_1)$ representing all such parameters. In other words, the data is modeled as

$$y^{(i)} \mid \psi \quad \sim \quad \text{Bernoulli}\,(\psi), \quad \text{for } i = 1, \ldots, n \tag{6}$$

$$x_j^{(i)} \mid y^{(i)}, \boldsymbol{\phi} \quad \sim \quad \text{Bernoulli}\,(\phi_{y^{(i)},j}), \quad \text{for } i = 1, \ldots, n \text{ and } j = 1, \ldots, p \tag{7}$$

We use a hierarchical prior that expresses the possibility that some features may have almost the same distribution in the two classes. In detail, the prior has the following form:

$$\psi \quad \sim \quad \text{Beta}\,(f_1, f_0) \tag{8}$$

$$\alpha \quad \sim \quad \text{Inverse-Gamma}(a, b) \tag{9}$$

$$\theta_1, \ldots, \theta_p \quad \stackrel{\text{IID}}{\sim} \quad \text{Uniform}(0, 1) \tag{10}$$

$$\phi_{0,j},\, \phi_{1,j} \mid \alpha,\, \theta_j \quad \stackrel{\text{IID}}{\sim} \quad \text{Beta}\,(\alpha\theta_j,\, \alpha(1{-}\theta_j)), \quad \text{for } j = 1, \ldots, p \tag{11}$$

The hyperparameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_p)$ are used to introduce dependence between $\boldsymbol{\phi}_{0,j}$ and $\boldsymbol{\phi}_{1,j}$, with α controlling the degree of dependence. Features for which $\phi_{0,j}$ and $\phi_{1,j}$ differ greatly are more relevant to predicting the response. When α is small, the variance of the Beta distribution in (11), which is $\theta_j\,(1{-}\theta_j)\,/\,(\alpha{+}1)$, is large, and many features are likely to have predictive power, whereas when α is large, it is likely that most features will be of little use in predicting the response, since $\phi_{0,j}$ and $\phi_{1,j}$ are likely to be almost equal. We chose an Inverse-Gamma prior for α (with density function proportional to $\alpha^{-(1+a)}\exp(-b/\alpha)$) because it has a heavy upward tail, allowing for the possibility that α is large. Our method of correcting selection bias will have the effect of modifying the likelihood in a way that favors larger values for α than would result from ignoring the effect of selection.

3.2 Integrating away ψ and $\boldsymbol{\phi}$

Although the above model is defined with ψ and $\boldsymbol{\phi}$ parameters for better conceptual understanding, computations are simplified by integrating them way analytically.

Integrating away ψ, the joint probability of $y^{\text{train}} = (y^{(1)}, \ldots, y^{(n)})$ is as follows, where $I(\,\cdot\,)$ is the indicator function, equal to 1 if the enclosed condition is true and 0 if it is false:

$$\begin{aligned} P(y^{\text{train}}) &= \int_0^1 \frac{\Gamma(f_0 + f_1)}{\Gamma(f_0)\Gamma(f_1)} \psi^{f_1} (1 - \psi)^{f_0}\, \psi^{\sum_{i=1}^{n} I(y^{(i)}=1)} (1 - \psi)^{\sum_{i=1}^{n} I(y^{(i)}=0)} d\psi & (12) \\ &= U\Big(f_0,\, f_1,\, \sum_{i=1}^{n} I\big(y^{(i)} = 0\big),\, \sum_{i=1}^{n} I\big(y^{(i)} = 1\big)\Big) & (13) \end{aligned}$$

The function U is defined as

$$U(f_0, f_1, n_0, n_1) \;\;=\;\; \frac{\Gamma(f_0+f_1)}{\Gamma(f_0)\Gamma(f_1)}\,\frac{\Gamma(f_0+n_0)\Gamma(f_1+n_1)}{\Gamma(f_0+f_1+n_0+n_1)} \;\;=\;\; \frac{\prod_{\ell=1}^{n_0}(f_0+\ell-1)\,\prod_{\ell=1}^{n_1}(f_1+\ell-1)}{\prod_{\ell=1}^{n_0+n_1}(f_0+f_1+\ell-1)} \tag{14}$$

The products above have the value one when the upper limits of n_0 or n_1 are zero. The joint probability of y^{train} and the response, y^*, for a test case is similar:

$$P(y^{\text{train}}, y^*) \;\;=\;\; U\Big(f_0,\, f_1,\, \sum_{i=1}^{n} I\big(y^{(i)}=0\big) + I(y^*=0),\, \sum_{i=1}^{n} I\big(y^{(i)}=1\big) + I(y^*=1)\Big) \tag{15}$$

Dividing $P(y^{\text{train}}, y^*)$ by $P(y^{\text{train}})$ gives

$$P(y^* \mid y^{\text{train}}) \;\;=\;\; \text{Bernoulli}\,(y^*; \hat{\psi}) \tag{16}$$

Here, $\text{Bernoulli}\,(y;\psi) \,=\, \psi^y\,(1-\psi)^{1-y}$ and $\hat{\psi} \,=\, (f_1+N_1)\,/\,(f_0+f_1+n)$, with $N_y = \sum_{\ell=1}^{n} I(y^{(\ell)}=y)$. Note that $\hat{\psi}$ is just the posterior mean of ψ based on $y^{(1)}, \ldots, y^{(n)}$.

Similarly, integrating over $\phi_{0,j}$ and $\phi_{1,j}$, we find that

$$P(x_j^{\text{train}} \mid \theta_j,\, \alpha,\, y^{\text{train}}) \;\;=\;\; \prod_{y=0}^{1} U(\alpha\theta_j,\, \alpha(1-\theta_j),\, O_{y,j},\, I_{y,j}) \tag{17}$$

where $O_{y,j} \;=\; \sum_{i=1}^{n} I(y^{(i)}=y,\, x_j^{(i)}=0)$ and $I_{y,j} \;=\; \sum_{i=1}^{n} I(y^{(i)}=y,\, x_j^{(i)}=1)$.

With ψ and $\boldsymbol{\phi}$ integrated out, we need deal only with the remaining parameters, α and $\boldsymbol{\theta}$. Note that after eliminating ψ and the $\boldsymbol{\phi}$, the cases are no longer independent (though they are exchangeable). However, conditional on the responses, y^{train}, and on α, the values of different features are still independent. This is crucial to the efficiency of the computations described below.

3.3 Predictions for test cases

We first describe how to predict the class for a test case when we are either using all features, or using a subset of features without any attempt to correct for selection bias. We then consider how to make predictions using our method of correcting for selection bias.

Suppose we wish to predict the response, y^*, in a test case for which we know the retained features $\boldsymbol{x}_{1:k}^* \,=\, (\boldsymbol{x}_1^*, \cdots, \boldsymbol{x}_k^*)$ (having renumbered features as necessary). For this, we need the following predictive probability:

$$P(y^* \,|\, \boldsymbol{x}_{1:k}^*,\, \boldsymbol{x}_{1:k}^{\text{train}},\, y^{\text{train}}) \;\;=\;\; \frac{P(y^* \,|\, y^{\text{train}})\, P(\boldsymbol{x}_{1:k}^* \,|\, y^*,\, \boldsymbol{x}_{1:k}^{\text{train}},\, y^{\text{train}})}{\sum_{y=0}^{1} P(y^*=y \,|\, y^{\text{train}})\, P(\boldsymbol{x}_{1:k}^* \,|\, y^*=y,\, \boldsymbol{x}_{1:k}^{\text{train}},\, y^{\text{train}})} \tag{18}$$

Ie, we evaluate the numerator above for $y^*=0$ and $y^*=1$, then divide by the sum to obtain the predictive probabilities. The first factor in the numerator, $P(y^* \,|\, y^{\text{train}})$, is given by equation (16).

It is sufficient to obtain the second factor up to a proportionality constant that doesn't depend on y^*, as follows:

$$P(\boldsymbol{x}^*_{1:k} \mid y^*, \boldsymbol{x}^{\rm train}_{1:k}, y^{\rm train}) \;=\; \frac{P(\boldsymbol{x}^*_{1:k}, x^{\rm train}_{1:k} \mid y^*, y^{\rm train})}{P(x^{\rm train}_{1:k} \mid y^{\rm train})} \;\propto\; P(\boldsymbol{x}^*_{1:k}, x^{\rm train}_{1:k} \mid y^*, y^{\rm train}) \tag{19}$$

This can be computed by integrating over α, noting that conditional on α the features are independent:

$$\begin{aligned} P(\boldsymbol{x}^*_{1:k}, x^{\rm train}_{1:k} \mid y^*, y^{\rm train}) &= \int P(\alpha)\, P(\boldsymbol{x}^*_{1:k}, x^{\rm train}_{1:k} \mid \alpha, y^*, y^{\rm train})\, d\alpha & (20)\\ &= \int P(\alpha) \prod_{j=1}^{k} P(\boldsymbol{x}^*_j, x^{\rm train}_j \mid \alpha, y^*, y^{\rm train})\, d\alpha & (21) \end{aligned}$$

Each factor in the product above is found by using equation (17) and integrating over θ_j:

$$\begin{aligned} P(\boldsymbol{x}^*_j, x^{\rm train}_j \mid \alpha, y^*, y^{\rm train}) &= \int_0^1 P(\boldsymbol{x}^*_j \mid \theta_j, \alpha, \boldsymbol{x}^{\rm train}_j, y^{\rm train}, y^*)\, P(\boldsymbol{x}^{\rm train}_j \mid \theta_j, \alpha, y^{\rm train})\, d\theta_j & (22)\\ &= \int_0^1 \text{Bernoulli}\,(\boldsymbol{x}^*_j; \hat\phi_{y^*,j}) \prod_{y=0}^{1} U(\alpha\theta_j, \alpha(1-\theta_j), I_{y,j}, O_{y,j})\, d\theta_j & (23) \end{aligned}$$

where $\hat\phi_{y^*,j} = (\alpha\theta_j + I_{y^*,j}) \,/\, (\alpha + N_{y^*})$, the posterior mean of $\phi_{y^*,j}$ given α and θ_j.

When using k features selected from a larger number, p, the predictions above, which are conditional on only $x^{\rm train}_{1:k}$ and $y^{\rm train}$, are not correct — we should also condition on the event, $\mathcal{S}$, that $|\text{COR}(y^{\rm train}, x^{\rm train}_j)| \le \gamma$ for $j = k+1, \ldots, p$. We need to modify the predictive probability of equation (18) by replacing $P(\boldsymbol{x}^*_{1:k} \mid y^*, \boldsymbol{x}^{\rm train}_{1:k}, y^{\rm train})$ with $P(\boldsymbol{x}^*_{1:k} \mid y^*, \boldsymbol{x}^{\rm train}_{1:k}, y^{\rm train}, \mathcal{S})$, which is proportional to $P(\boldsymbol{x}^*_{1:k}, \boldsymbol{x}^{\rm train}_{1:k}, \mathcal{S} \mid y^*, y^{\rm train})$. Analogously to equations (20) and (21), we obtain

$$\begin{aligned} P(\boldsymbol{x}^*_{1:k}, x^{\rm train}_{1:k}, \mathcal{S} \mid y^*, y^{\rm train}) &= \int P(\alpha)\, P(\boldsymbol{x}^*_{1:k}, x^{\rm train}_{1:k}, \mathcal{S} \mid \alpha, y^*, y^{\rm train})\, d\alpha & (24)\\ &= \int P(\alpha)\, P(\mathcal{S} \mid \alpha, y^{\rm train}) \prod_{j=1}^{k} P(\boldsymbol{x}^*_j, x^{\rm train}_j \mid \alpha, y^*, y^{\rm train})\, d\alpha & (25) \end{aligned}$$

The factors for the k retained features are computed as before, using equation (23). The additional correction factor that is needed (presented earlier as equation (5)) is

$$\begin{aligned} P(\mathcal{S} \mid \alpha, y^{\rm train}) &= \prod_{j=k+1}^{p} P(|\text{COR}(y^{\rm train}, x^{\rm train}_j)| \le \gamma \mid \alpha, y^{\rm train}) & (26)\\ &= \Big[P(|\text{COR}(y^{\rm train}, x^{\rm train}_t)| \le \gamma \mid \alpha, y^{\rm train}) \Big]^{p-k} & (27) \end{aligned}$$

where t is any of the omitted features, all of which have the same probability of having a small correlation with y. We discuss how to compute this adjustment factor in the next section.

To see intuitively why this adjustment factor will correct for selection bias, recall that as discussed in Section (3.1), when α is small, features will be more likely to have a strong relationship with the response. If the likelihood of α is based only on the selected features, which have shown high correlations with the response in the training dataset, it will favor values of α that are inappropriately small. Multiplying by the adjustment factor, which favors larger values for α, undoes this bias.

We compute the integrals over α in equations (21) and (25) by numerical quadrature. We use the midpoint rule, applied to $u = F^{-1}(\alpha)$, where F^{-1} is the inverse cumulative distribution function for the Inverse-Gamma(a, b) prior for α. The prior for u is uniform over $(0, 1)$, and so needn't be explicitly included in the integrand. With K points for the midpoint rule, the effect is that we average the value of the integrand, without the prior factor, for values of α that are the $0.5/K, 1.5/K, \ldots, 1 - 0.5/K$ quantiles of its Inverse-Gamma prior. For each α, we use Simpson's Rule to compute the one-dimensional integrals over θ_j in equation (23).

3.4 Computation of the adjustment factor

Our remaining task is to compute the adjustment factor of equation (27), which depends on the probability that a feature will have correlation less than γ in absolute value. Computing this seems difficult — we need to sum the probabilities of $\boldsymbol{x}_t^{\text{train}}$ given y^{train}, α and θ_t over all configurations of $\boldsymbol{x}_t^{\text{train}}$ for which $|\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \leq \gamma$ — but the computation can be simplified by noticing that $\text{COR}(x_t^{\text{train}}, y^{\text{train}})$ can be written in terms of $I_0 = \sum_{i=1}^n I(y^{(i)} = 0,\, x_t^{(i)} = 1)$ and $I_1 = \sum_{i=1}^n I(y^{(i)} = 1,\, x_t^{(i)} = 1)$, as follows:

$$\text{COR}(x_t^{\text{train}},\, y^{\text{train}}) = \frac{\sum_{i=1}^{n} \left(y^{(i)} - \overline{y}\right) x_t^{(i)}}{\sqrt{\sum_{i=1}^{n} \left(y^{(i)} - \overline{y}\right)^2} \sqrt{\sum_{i=1}^{n} \left(x_t^{(i)} - \bar{x}_t\right)^2}} \tag{28}$$

$$= \frac{(0 - \overline{y})\, I_0 \;+\; (1 - \overline{y})\, I_1}{\sqrt{n\overline{y}(1-\overline{y})}\, \sqrt{I_0 + I_1 - (I_0 + I_1)^2/n}} \tag{29}$$

We write the above as $\text{Cor}(I_0, I_1, \overline{y})$, taking n as known. This function is defined for $0 \leq I_0 \leq n(1-\overline{y})$ and $0 \leq I_1 \leq n\overline{y}$.

Fixing n, $\overline{y}$, and γ, we can define the following sets of values for I_0 and I_1 (for some feature x_t) in terms of the resulting correlation with y:

$$L_0 = \{\, (I_0, I_1) \;:\; \text{Cor}(I_0, I_1, \overline{y}) = 0 \,\} \tag{30}$$

$$L_+ = \{\, (I_0, I_1) \;:\; 0 < \text{Cor}(I_0, I_1, \overline{y}) \leq \gamma \,\} \tag{31}$$

$$L_- = \{\, (I_0, I_1) \;:\; -\gamma \leq \text{Cor}(I_0, I_1, \overline{y}) < 0 \,\} \tag{32}$$

$$H_+ = \{\, (I_0, I_1) \;:\; \gamma < \text{Cor}(I_0, I_1, \overline{y}) \,\} \tag{33}$$

$$H_- = \{\, (I_0, I_1) \;:\; \text{Cor}(I_0, I_1, \overline{y}) < -\gamma \,\} \tag{34}$$

A feature will be discarded if $(I_0, I_1) \in L_- \cup L_0 \cup L_+$ and retained if $(I_0, I_1) \in H_- \cup H_+$. These sets are illustrated in Figure 1.

I_1 \ I_0	0	1	2	3	4	5	6	7	8
14	+1.00	+0.90	+0.81	+0.72	+0.62	+0.53	+0.42	+0.29	0.00
13	+0.91	+0.80	+0.70	+0.60	+0.49	+0.38	+0.25	+0.09	−0.16
12	+0.83	+0.72	+0.61	+0.50	+0.39	+0.27	+0.13	−0.03	−0.24
11	+0.76	+0.64	+0.52	+0.41	+0.30	+0.17	+0.04	−0.11	−0.30
10	+0.69	+0.57	+0.45	+0.33	+0.21	+0.09	−0.04	−0.18	−0.36
9	+0.63	+0.50	+0.38	+0.26	+0.14	+0.02	−0.11	−0.25	−0.41
8	+0.57	+0.44	+0.31	+0.19	+0.07	−0.05	−0.18	−0.31	−0.46
7	+0.52	+0.38	+0.24	+0.12	0.00	−0.12	−0.24	−0.37	−0.52
6	+0.46	+0.31	+0.18	+0.05	−0.07	−0.19	−0.31	−0.44	−0.57
5	+0.41	+0.25	+0.11	−0.02	−0.14	−0.26	−0.38	−0.50	−0.63
4	+0.36	+0.18	+0.04	−0.09	−0.21	−0.33	−0.45	−0.57	−0.69
3	+0.30	+0.11	−0.04	−0.17	−0.30	−0.41	−0.52	−0.64	−0.76
2	+0.24	+0.03	−0.13	−0.27	−0.39	−0.50	−0.61	−0.72	−0.83
1	+0.16	−0.09	−0.25	−0.38	−0.49	−0.60	−0.70	−0.80	−0.91
0	0.00	−0.29	−0.42	−0.53	−0.62	−0.72	−0.81	−0.90	−1.00

Figure 1: The Cor function for a dataset with $n = 22$ and $\overline{y} = 14/22$. The values of $\mathrm{Cor}(I_0, I_1, \overline{y})$ are shown for the valid range of I_0 and I_1. Using $\gamma = 0.2$, the values of (I_0,I_1) in L_0 are shown in dark grey, those in L_- or L_+ in medium grey, and those in H_- or H_+ in light grey.

We can write the probability needed in equation (27) using either L_-, L_0, and L_+ or H_- and H_+. We will take the latter approach here, as follows:

$$P(\,|\mathrm{COR}(x_t^{\mathrm{train}}, y^{\mathrm{train}})| \le \gamma \mid \alpha,\, y^{\mathrm{train}}) \;=\; 1 \;-\; P(\,(I_0, I_1) \,\in\, H_- \cup H+ \;\mid \alpha,\, y^{\mathrm{train}}) \tag{35}$$

$$= \; 1 \;-\; \sum_{\substack{(I_0,I_1)\,\in \\ H_-\cup H_+}} P(I_0,\, I_1 \mid \alpha,\, y^{\mathrm{train}}) \tag{36}$$

We can now exploit symmetries of the prior and of the Cor function to speed up computation. First, note that $\mathrm{Cor}(I_0, I_1, \overline{y}) \;=\; -\mathrm{Cor}(n(1-\overline{y})-I_0, n\overline{y}-I_1, \overline{y})$, as can be derived from equation (29), or by simply noting that swapping the feature values (0 and 1) should change only the sign of the correlation. The one-to-one mapping $(I_0, I_1) \to (n(1-\overline{y}) - I_0, n\overline{y} - I_1)$, which maps H_- and H_+ and vice versa (similarly for L_- and L_+), therefore leaves Cor unchanged. The priors for θ and ϕ (see (10) and (11)) are symmetrical with respect to the class labels 0 and 1, so the prior probability of $(I_0,\, I_1)$ is the same as that of $(n(1-\overline{y}) - I_0,\, n\overline{y} - I_1)$. We can therefore rewrite equation (36) as

$$P(\,|\mathrm{COR}(x_t^{\mathrm{train}}, y^{\mathrm{train}})| \le \gamma \mid \alpha,\, y^{\mathrm{train}}) \;=\; 1 \;-\; 2 \sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, y^{\mathrm{train}}) \tag{37}$$

At this point we write the probabilities for I_0 and I_1 in terms of an integral over θ_t, and then swap the order of summation and integration, obtaining

$$\sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, y^{\mathrm{train}}) \;=\; \int_0^1 \sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, \theta_t,\, y^{\mathrm{train}})\; d\theta_t \tag{38}$$

The integral over θ_t can be approximated using some one-dimensional numerical quadrature method (we use Simpson's Rule), provided we can evaluate the integrand.

The sum over H_+ can easily be delineated because $\text{Cor}(I_0, I_1, \overline{y})$ is a monotonically decreasing function of I_0, and a monotonically increasing function of I_1, as may be confirmed by differentiating with respect to I_0 and I_1. Let b_0 be the smallest value of I_1 for which $\text{Cor}(0, I_1, \overline{y}) > \gamma$. Taking the ceiling of the solution of $\text{Cor}(0, I_1, \overline{y}) = \gamma$, we find that $b_0 = \lceil 1/(1/n + (1-\bar{y})/(n\bar{y}\gamma^2)) \rceil$. For $b_0 \le I_1 \le n\overline{y}$, let r_{I_1} be the largest value of I_0 for which $\text{Cor}(I_0, I_1, \overline{y}) > \gamma$. We can write

$$\sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \;=\; \sum_{I_1=b_0}^{n\overline{y}} \sum_{I_0=0}^{r_{I_1}} P(I_0,\, I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \tag{39}$$

Given α and θ_t, I_0 and I_1 are independent, so we can reduce the computation needed by rewriting the above expression as follows:

$$\sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \;=\; \sum_{I_1=b_0}^{n\overline{y}} P(I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \sum_{I_0=0}^{r_{I_1}} P(I_0 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \tag{40}$$

Note that the inner sum can be updated from one value of I_1 to the next by just adding any additional terms needed. This calculation therefore requires $1 + n\overline{y} - b_0 \le n$ evaluations of $P(I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}})$ and $1 + r_{n\overline{y}} \le n$ evaluations of $P(I_0 \mid \alpha,\, \theta_t,\, y^{\text{train}})$.

To compute $P(I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}})$, we multiply the probability of any particular value for x_t^{train} in which there are I_1 cases with $y = 1$ and $x_t = 1$ by the number of ways this can occur. The probabilities are found by integrating over $\phi_{0,t}$ and $\phi_{1,t}$, as described in Section 3.2. The result is

$$P(I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \;=\; \binom{n\overline{y}}{I_1} U(\alpha\theta_t,\, \alpha(1-\theta_t),\, I_1,\, n\overline{y} - I_1) \tag{41}$$

Similarly,

$$P(I_0 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \;=\; \binom{n(1-\overline{y})}{I_0} U(\alpha\theta_t,\, \alpha(1-\theta_t),\, I_0,\, n(1-\overline{y}) - I_0) \tag{42}$$

One can easily derive simple expressions for $P(I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}})$ and $P(I_0 \mid \alpha,\, \theta_t,\, y^{\text{train}})$ in terms of $P(I_1 - 1 \mid \alpha,\, \theta_t,\, y^{\text{train}})$ and $P(I_0 - 1 \mid \alpha,\, \theta_t,\, y^{\text{train}})$, which avoid the need to compute gamma functions or large products for each value of I_0 or I_1 when these values are used sequentially, as in equation (40).

4 A Simulation Experiment

In this section, we use a dataset generated from the naive Bayes model defined in Section 3.1 to demonstrate the lack of calibration that results when only a subset of features is used, without correcting for selection bias. We show that our bias-correction method eliminates this lack of calibration. We will also see that for the naive Bayes model only a small amount of extra computation time is needed to obtain the adjustment factor needed by our method.

Fixing $\alpha = 300$, and $p = 10000$, we used equations (7), (10) and (11) to generate a set of 200 training cases and a set of 2000 test cases, both having equal numbers of cases with $y = 0$ and $y = 1$. We then selected four subsets of features, containing 1, 10, 100, and 1000 features, based on the absolute values of the sample correlations of the features with y. The smallest correlation (in absolute value) of a selected feature with the class was 0.36, 0.27, 0.21, and 0.13 for these four subsets. These are the values of γ used by the bias correction method when computing the adjustment factor of equation (27). Figure 2 shows the absolute value of the sample correlation in the training set of all 10000 features, plotted against the sample correlation in the test set. As can be seen, the high sample correlation of many selected features in the training set is partly or wholely a matter of chance, with the sample correlation in the test set (which is close to the real correlation) often being much less. The role of chance is further illustrated by the fact that the feature with highest sample correlation in the test set is not even in the top 1000 by sample correlation in the training set.

For each number of selected features, we fit this data using the naive Bayes model with the prior for ψ (equation (8)) having $f_0 = f_1 = 1$ and the prior for α (equation (9)) having shape parameter $a = 0.5$ and rate parameter $b = 5$. We then made predictions for the test cases using the methods described in Section 3.3. The "uncorrected" method, based on equation (18), makes no attempt to correct for the selection bias, whereas the "corrected" method, with the modification of equation (25), produces predictions that account for the procedure used to select the subset of features. We also made predictions using all 10000 features, for which bias correction is unnecessary.

We compared the predictive performance of the corrected method with the uncorrected method in several ways. First, we looked at the error rate when classifying test cases by thresholding the predictive probabilities at 1/2. As can be seen in Figure 3, there is little difference in the error rates with and without correction for bias. However, the methods differ drastically in terms of the *expected* error rate — the error rate we would expect based on the predictive probabilities for the test cases, equal to $(1/N) \sum_i \hat{p}^{(i)} I(\hat{p}^{(i)} < 0.5) \ + \ (1-\hat{p}^{(i)}) I(\hat{p}^{(i)} \geq 0.5)$, where $\hat{p}^{(i)}$ is the predictive probability of class 1 for test case i. The predictive probabilities produced by the uncorrected method would lead us to believe that we would have a much lower error rate than the actual performance. In contrast, the expected error rates based on the predictive probabilities produced using bias correction closely match the actual error rates.

Two additional measures of predictive performance are shown in Figure 4. One measure of performance is minus the average log probability of the correct class in the N test cases, which is $-(1/N) \sum_{i=1}^{N} [y^{(i)} \log(\hat{p}^{(i)}) + (1-y^{(i)}) \log(1-\hat{p}^{(i)})]$. This measure heavily penalizes test cases where the actual class has a predictive probability near zero. Another measure, less sensitive to such drastic errors, is the average squared error between the actual class (0 or 1) and the probability of class 1, given by $(1/N) \sum_{i=1}^{N} (y^{(i)} - \hat{p}^{(i)})^2$. The corrected method outperforms the uncorrected method by both these measures, with the difference being greater for minus average log probability. Interestingly, performance of the uncorrected method actually gets worse when going from 1 feature to 10 features. This may be because the single feature with highest sample correlation with the response does have a strong relationship with the response (as may be likely in general), whereas some other of the top 10 features by sample correlation have little or no real relationship.

We also looked in more detail at how well calibrated the predictive probabilities were. Table 1

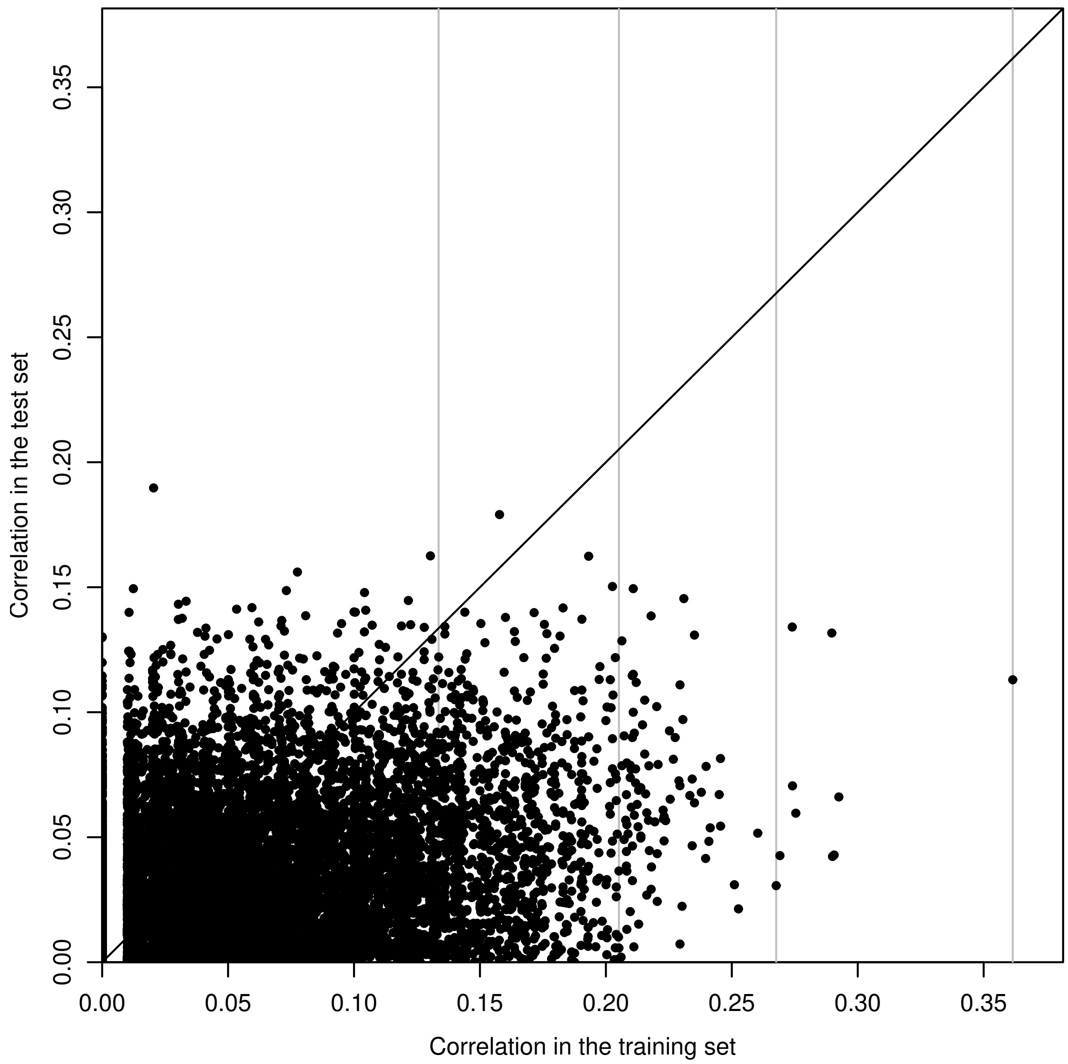


Figure 2: The absolute value of the sample correlation of each feature with the binary response, in the training set, and in the test set. Each dot represents one of the 10000 binary features. The training set correlations of the 1st, 10th, 100th, and 1000th most correlated features are marked by vertical lines.

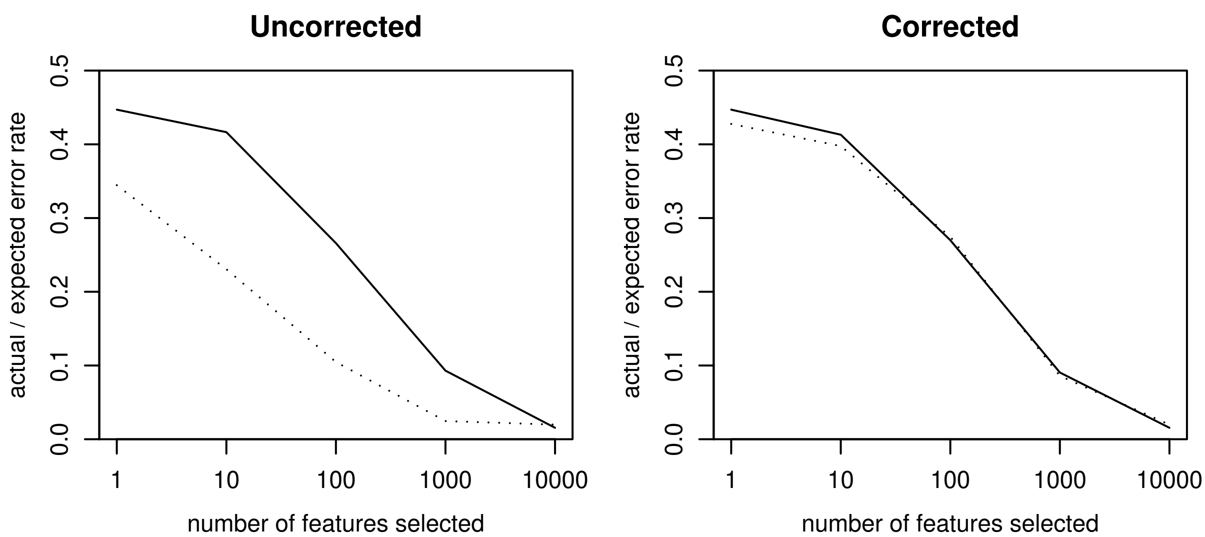


Figure 3: Actual and expected error rates with varying numbers of features selected, with and without correction for selection bias. The solid line is the actual error rate on test cases. The dotted line is the error rate that would be expected based on the predictive probabilities.

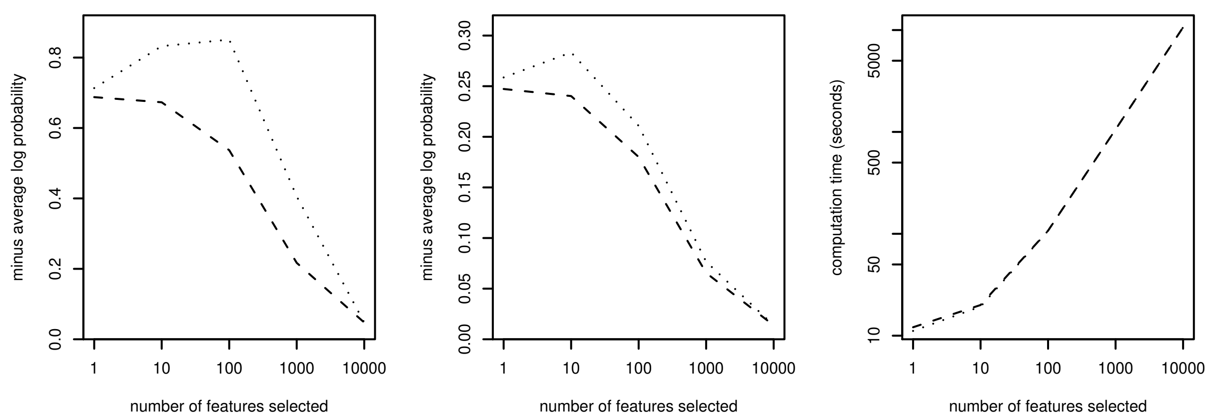


Figure 4: Performance in terms of average minus log probability and average squared error, and computation time, with varying numbers of features selected, with and without correction for selection bias. The left plot shows minus the average log probability of the correct class for test cases, with 1, 10, 100, 1000, and all 10000 features selected. The dashed line is with bias correction, the dotted line without. The middle plot is similar, but shows average squared error on test cases. The right plot shows the computation time needed for the methods (the two lines almost coincide). Note that when all 10000 features are used, there is no difference between the corrected and uncorrected methods.

	1 feature selected out of 10000						10 features selected out of 10000					
	Corrected			Uncorrected			Corrected			Uncorrected		
Category	#	Pred	Actual	#	Pred	Actual	#	Pred	Actual	#	Pred	Actual
0.0 - 0.1	0	–	–	0	–	–	0	–	–	237	0.046	0.312
0.1 - 0.2	0	–	–	0	–	–	3	0.174	0.000	349	0.149	0.444
0.2 - 0.3	0	–	–	0	–	–	126	0.270	0.294	68	0.249	0.500
0.3 - 0.4	0	–	–	1346	0.384	0.461	467	0.360	0.420	300	0.360	0.443
0.4 - 0.5	1346	0.446	0.461	0	–	–	566	0.462	0.461	189	0.443	0.487
0.5 - 0.6	0	–	–	0	–	–	461	0.554	0.566	48	0.546	0.417
0.6 - 0.7	654	0.611	0.581	0	–	–	276	0.643	0.616	238	0.650	0.588
0.7 - 0.8	0	–	–	654	0.736	0.581	97	0.733	0.742	180	0.737	0.567
0.8 - 0.9	0	–	–	0	–	–	4	0.825	0.750	192	0.864	0.609
0.9 - 1.0	0	–	–	0	–	–	0	–	–	199	0.943	0.668

	100 features selected out of 10000						1000 features selected out of 10000					
	Corrected			Uncorrected			Corrected			Uncorrected		
Category	#	Pred	Actual	#	Pred	Actual	#	Pred	Actual	#	Pred	Actual
0.0 - 0.1	155	0.067	0.077	717	0.017	0.199	774	0.018	0.027	954	0.004	0.066
0.1 - 0.2	247	0.151	0.162	133	0.150	0.391	97	0.143	0.165	28	0.149	0.500
0.2 - 0.3	220	0.247	0.286	70	0.251	0.429	63	0.243	0.302	13	0.248	0.846
0.3 - 0.4	225	0.352	0.356	68	0.351	0.515	48	0.346	0.438	17	0.349	0.412
0.4 - 0.5	237	0.450	0.494	58	0.451	0.500	45	0.446	0.600	14	0.449	0.786
0.5 - 0.6	227	0.545	0.586	78	0.552	0.603	44	0.547	0.614	16	0.546	0.375
0.6 - 0.7	202	0.650	0.728	77	0.654	0.532	53	0.647	0.698	16	0.667	0.812
0.7 - 0.8	214	0.749	0.785	80	0.746	0.662	81	0.755	0.815	22	0.751	0.636
0.8 - 0.9	182	0.847	0.857	98	0.852	0.633	124	0.854	0.863	25	0.865	0.560
0.9 - 1.0	91	0.935	0.923	621	0.979	0.818	671	0.977	0.982	895	0.995	0.946

	Complete data		
Category	#	Pred	Actual
0.0 - 0.1	964	0.004	0.006
0.1 - 0.2	21	0.145	0.238
0.2 - 0.3	8	0.246	0.375
0.3 - 0.4	10	0.342	0.300
0.4 - 0.5	12	0.436	0.500
0.5 - 0.6	7	0.544	1.000
0.6 - 0.7	20	0.656	1.000
0.7 - 0.8	13	0.743	0.846
0.8 - 0.9	22	0.851	0.818
0.9 - 1.0	923	0.994	0.998

Table 1: Comparison of calibration for predictions found with and without correction for selection bias, on data simulated from the binary naive Bayes model. Results are shown with four subsets of features and with the complete data (for which no correction is necessary). The test cases were divided into 10 categories by the first decimal of the predictive probablity of class 1. The table shows the number of test cases in each category for each method ("#"), the average predictive probability of class 1 for cases in that category ("Pred"), and the actual fraction of these cases that were in class 1 ("Actual").

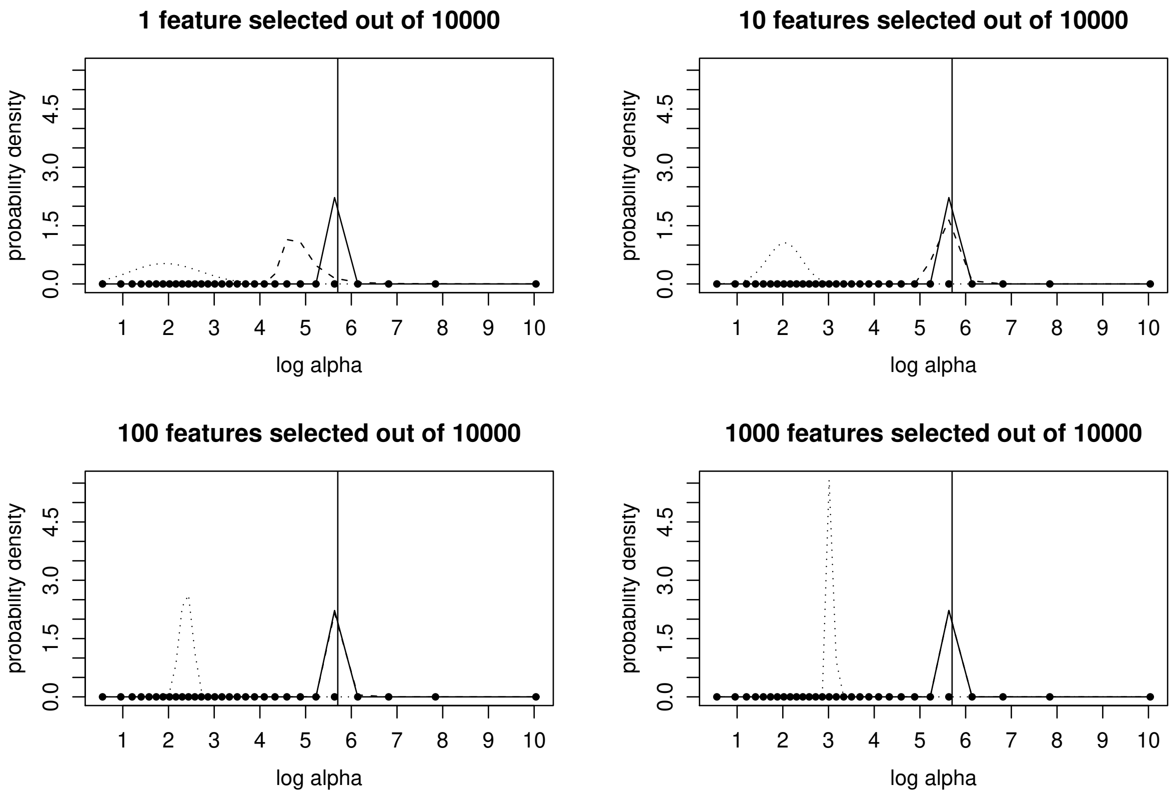


Figure 5: Posterior distributions of $\log(\alpha)$ for the simulated data, with different numbers of features selected. The true value of $\log(\alpha)$ is 5.7, shown by the vertical line. The solid line is the posterior density using all features. For each number of selected features, the dashed line is the posterior density including the factor that corrects for selection bias; the dotted line is the posterior density without bias correction. The dashed and solid lines overlap in the bottom two graphs. The dots mark the values of $\log(\alpha)$ used to approximate the density, at the $0.5/K, 1.5/K, \ldots, (K-0.5)/K$ quantiles of the prior distribution (where $K = 30$). The probabilities of x^{train} at each of these values for α were computed, rescaled to sum to K, and finally multiplied by the Jacobian, $\alpha P(\alpha)$, to obtain the approximation to the posterior density of $\log(\alpha)$.

shows the average predictive probability for class 1 and the actual fraction of cases in class 1 for test cases grouped according to the first decimal of their predictive probabilities, for both the uncorrected and the corrected methods. Results are shown using subsets of 1, 10, 100, and 1000 features, and using all features. We see that the uncorrected method produces overconfident predictive probabilities, either too close to zero or too close to one. The corrected method avoids such bias (the values for "Pred" and "Actual" are much closer), showing that it is well calibrated.

The biased predictions of the uncorrected method result from an incorrect posterior distribution for α, as illustrated in Figure 5. Without bias correction, the posterior based on only the selected features incorrectly favours values of α smaller than the true value of 300. Multiplying by the adjustment factor corrects this bias in the posterior distribution.

Our software (available from `http://www.utstat.utoronto.ca/~longhai`) is written in the R language, with some functions for intensive computations such as numerical integration and computation of the adjustment factor written in C for speed. We approximated the integral with respect to α using the midpoint rule with $K = 30$ values for $F^{-1}(\alpha)$, as discussed at the end of Section 3.3. The integrals with respect to θ in equations (23) and (38) were approximated using Simpson's Rule, evaluating θ at 21 points.

Computation times for each method (on a 1.2 GHz UltraSPARC III processor) are shown on the right in Figure 4. The corrected method is almost as fast as the uncorrected method, since the time to compute the adjustment factor is negligible compared to the time spent computing the integrals over θ_j for the selected features. Accordingly, considerable time can be saved by selecting a subset of features, rather than using all of them, without introducing an optimistic bias, though some accuracy in predictions may of course be lost when we discard the information contained in the unselected features.

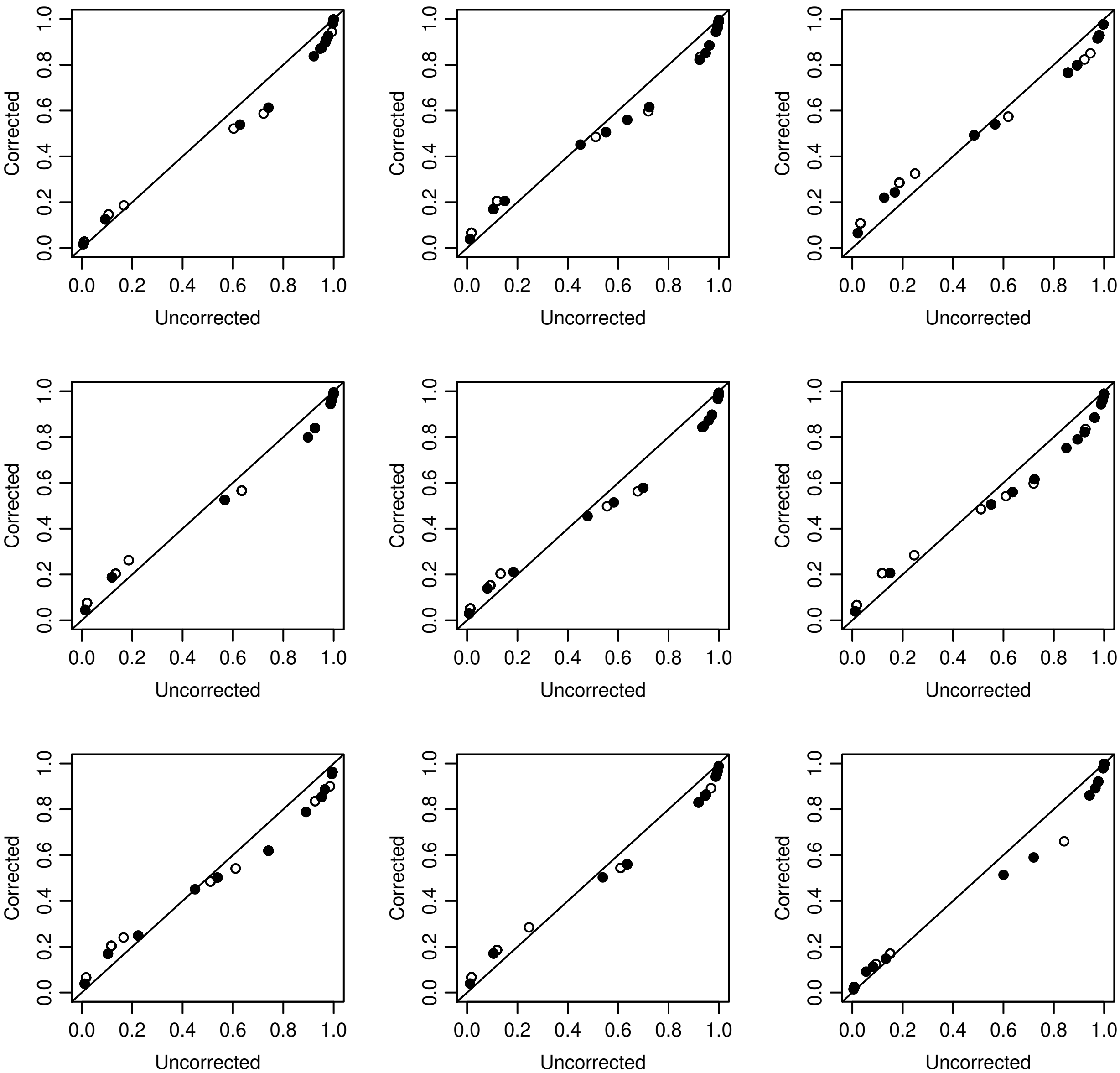
5 A test using gene expression data

We also tested our method using a publicly available dataset on gene expression in normal and cancerous human colon tissue. This dataset contains the expression levels of 6500 genes in 40 cancerous and 22 normal colon tissues, measured using the Affymetrix technology. The dataset is available at `http://geneexpression.cinj.org/∼notterman/affyindex.html`. We used only the 2000 genes with highest minimal intensity, as selected by Alon, Barkai, Notterman, Gish, Mack, and Levine (1999). In order to apply the binary naive Bayes model to the data, we transformed the real-value data into binary data by thresholding at the median, separately for each feature.

We divided these 2000 genes randomly into 10 equal groups, producing 10 smaller datasets, each with 200 binary features, as well as the binary class (normal/cancerous). We applied the corrected and uncorrected methods separately to each of these 10 datasets, allowing some assessment of variability when comparing performance. For each of these 10 datasets, we used leave-one-out cross validation to obtain predictive probabilities for the class in the 62 cases. In this cross-validation procedure, we left out each of the 62 cases in turn, selected the five features with the largest sample correlation with the class (in absolute value), and found the predictive probability for the left-out case using the binary naive Bayes model, with and without bias correction. The absolute value of the correlation of the last selected feature with the class was always around 0.5. We used the same prior distribution, and the same computational methods, as for the demonstration in Section 4.

Figure 6 plots the predictive probabilities of class 1 for all cases, with each of the 10 subsets of features. The tendency of the uncorrected method to produce more extreme probabilities (closer to 0 and 1) is clear. However, when the predictive probability is close to 0.5, there is little difference between the corrected and uncorrected methods. Accordingly, the two methods usually classify cases the same way, if classification is done by thresholding the predictive probability at 0.5, and have very similar error rates. (The overall average error rate is 0.194 for the uncorrected method and 0.182 for the corrected method.) Note, however, that correcting for bias would have a substantial effect if cases were classified by thresholding the predictive probability at some value other than 0.5, as would be appropriate if the consequences of an error are different for the two classes.

Figure 7 compares the two methods in terms of average minus log probability of the correct class and in terms of average squared error. From these plots it is clear that bias correction improves the



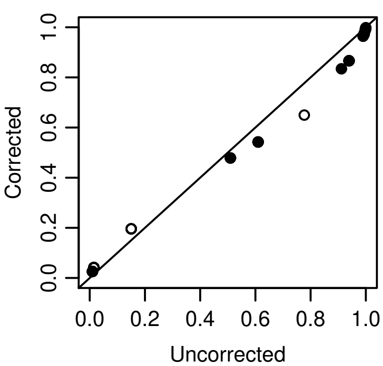


Figure 6: Scatterplots of the predictive probabilities of class 1 for the 10 subsets drawn from the colon cancer gene expression data, with and without correction for selection bias. Black circles are cases that are actually in class 1 (cancer); hollow circles are cases that are actually in class 0. Note that many cases with predictive probabilities close to 0 or 1 may overlap.

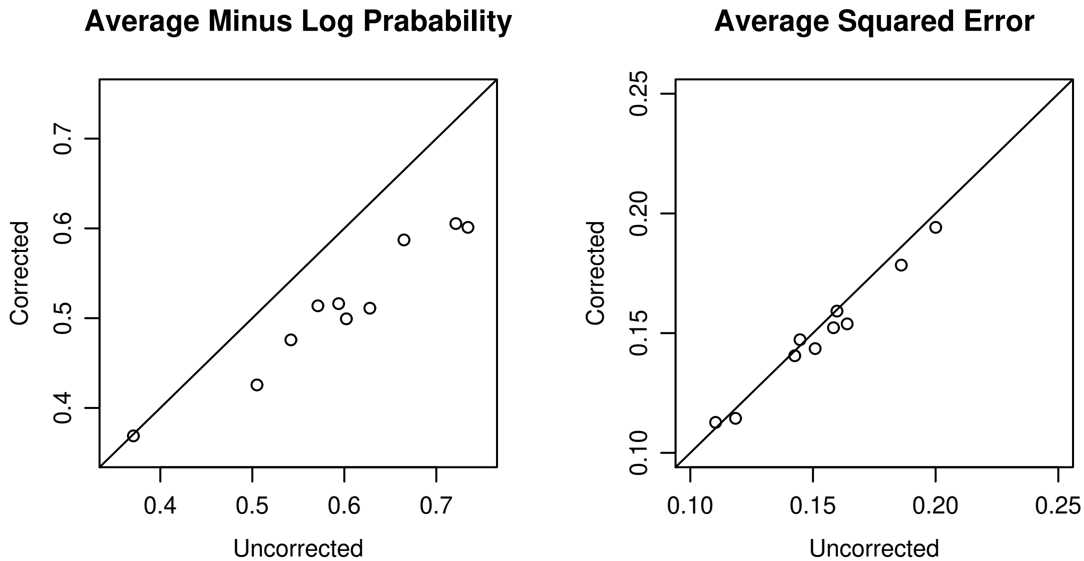


Figure 7: Scatterplots of the average minus log probability of the correct class and of the average squared error (assessed by cross validation) when using the 10 subsets of features for the colon cancer gene expression data, with and without correcting for selection bias.

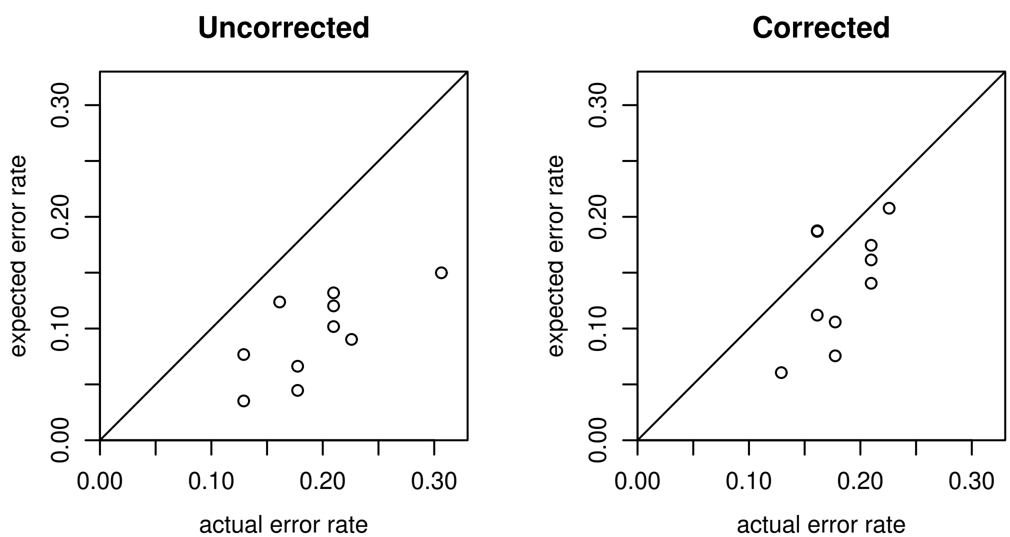


Figure 8: Actual versus expected error rates on the colon cancer datasets, with and without bias correction. Points are shown for each of the 10 subsets of features used for testing. In the plot on the right, two points above the diagonal are almost superimposed.

predictive probabilities. In terms of average minus log probability, the corrected method is better for all 10 datasets, and in terms of average squared error, the corrected method is better for 8 out of 10 datasets. (A paired t test with these two measures produced p-values of 0.00007 and 0.019 respectively.)

Finally, Figure 8 shows that our bias correction method reduces optimistic bias in the predictions. For each of the 10 datasets, this plot shows the actual error rate (in the leave-one-out cross-validation assessment) and the error rate expected from the predictive probabilities. For all ten datasets, the expected error rate with the uncorrected method is substantially less than the actual error rate. This optimistic bias is reduced in the corrected method, though it is not eliminated entirely. The remaining bias presumably results from the failure in this dataset of the naive Bayes assumption that features are independent within a class.

6 Conclusions and Future Work

We have proposed a Bayesian method for making well-calibrated predictions for a response variable when using a subset of features selected from a larger number based on some measure of dependency between the feature and the response. Our method results from applying the basic principle that predictive probabilities should be conditional on all available information — in this case, including the information that some features were discarded because they appear weakly related to the response variable. This information can only be utilized when using a model for the joint distribution of the response and the features, even though we are interested only in the conditional distribution of the response given the features.

We applied this method to naive Bayes models with binary features that are assumed to be independent conditional on the value of the binary response (class) variable. With these models, we can efficiently compute the adjustment factor needed to correct for selection bias. Crucially, we need only compute the probability that a single feature will exhibit low correlation with the response, and then raise this probability to the number of discarded features. When a large number of features are discarded, the time needed to compute the adjustment factor for bias correction is much less that the time that would have been needed to actually use these features. Substantial computation time can therefore be saved by discarding features that appear to have little relationship with the response.

Our general method can be applied to other models and other feature selection criteria, provided that the adjustment factor can be computed. Reasonably efficient computation may be possible when the features for a case are independent given the values for a set of latent variables, since the adjustment factor can then again be found by raising the probability that a single feature will be discarded to the number of features that were discarded. However, since the values for latent variables will not be known, the computations are more difficult than for the naive Bayes model. Markov chain Monte Carlo methods will generally be needed to sample for the values of the latent variables. (They may be required in any case for models more complex than the binary naive Bayes model considered in this paper.)

We have implemented such bias correction methods for two-component mixture models of binary data, and for factor analysis models, in which the features and the response are real valued. The required computations are feasible, but slower and more complex than for the naive Bayes model. We will report the details of these methods and their performance in follow-on papers. The practical utility of the bias correction method we describe would be much improved if methods for more efficiently computing the required adjustment factor could be found, which could be applied to a wide class of models.

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