Generalized Bayesian Quantification Learning

Jacob Fiksel*
Department of Biostatistics Johns Hopkins University
and
Abhirup Datta
Department of Biostatistics Johns Hopkins University
and
Agbessi Amouzou
Department of International Health Johns Hopkins University
and
Scott Zeger
Department of Biostatistics Johns Hopkins University

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Abstract

Quantification learning is the task of prevalence estimation for a test population using predictions from a classifier trained on a different population. Commonly used quantification methods either assume perfect sensitivity and specificity of the classifier, or use the training data to both train the classifier and also estimate its misclassification rates. These methods are inappropriate in the presence of dataset shift, when the misclassification rates in the training population are not representative of those for the test population. A recent Bayesian quantification model addresses dataset shift, but only allows for single-class (categorical) predictions, and assumes perfect knowledge of the true labels on a small number of instances from the test population. We propose a generalized Bayesian quantification learning (GBQL) approach that uses the entire compositional predictions from probabilistic classifiers and allows for uncertainty in true class labels for the limited labeled test data. Instead of positing a full model, we use a model-free Bayesian estimating equation approach to compositional data using Kullback-Liebler losses based only on a first-moment assumption. The idea will be useful in Bayesian compositional data analysis in general as it is robust to different generating mechanisms for compositional data and allows 0’s and 1’s in the compositional outputs thereby including categorical outputs as a special case. For the quantification problem, this estimating equation approach coherently links the losses for labeled and unlabeled test cases. We show how our method yields existing quantification approaches as special cases through different prior choices thereby providing an inferential framework around these approaches. This observation also enables using shrinkage towards these approaches via priors which stabilizes estimation in data-scarce settings. Extension to an ensemble GBQL that uses predictions from multiple classifiers yielding inference robust to inclusion of a poor classifier is discussed. We outline a fast and efficient Gibbs sampler using a rounding and coarsening approximation to the loss functions. For large sample settings, we establish posterior consistency of GBQL, which to our knowledge is the first result on consistency of a quantification approach in presence of local labeled data. Empirical performance of GBQL is demonstrated through simulations and analysis of real data with evident dataset shift.

Keywords: Bayesian, compositional data, estimating equations, machine learning, quantification.

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1 Introduction

Classifiers are most commonly developed with the goal of obtaining accurate predictions for individual units. However, in some applications, the objective is not individual level predictions, but rather to learn about population-level distributions of a given outcome. Examples include sentiment analysis for Twitter users (Giachanou and Crestani, 2016), estimating the prevalence of chronic fatigue syndrome (Valdez et al., 2018), and cause of death distribution estimation from verbal autopsies (King et al., 2008; McCormick et al., 2016; Serina et al., 2015; Byass et al., 2012; Miasnikof et al., 2015).

The task of predicting the population distribution of unobserved true outcomes (labels) based on observed covariates has been termed quantification (Forman, 2005; Bella et al., 2010; González et al., 2017; Pérez-Gállego et al., 2019) in the machine learning literature. Since the covariates are usually passed through a classifier to obtain predicted labels, quantification can be viewed as prevalence estimation using these predicted labels. Quantification requires building a classifier which can predict an outcome $y$ using (possibly high-dimensional) covariates $x$. This can be done by obtaining training data with observed outcomes $y$ and variables $x$ that can be used to train a classifier, or alternatively, creating a classifier based on expert knowledge (Kalter et al., 2015). In either case, the classifier is then used to predict labels in the test set representing the population of interest where we want to estimate the distribution of the categorical outcome $y$, but only observe $x$. The predicted classes (or probabilities) for individuals in the test set are then aggregated to obtain an estimate of the distribution of the outcome in this population, $p_{\text{test}}(y)$ (Forman, 2005).

Quantification is distinct from building a classifier algorithm. It also goes beyond the task of training a classifier to accurately predict individual labels, as common methods for quantification (reviewed in Section 2) adjust output from inaccurate classifiers to improve quantification (Forman, 2008; Bella et al., 2010). However, these adjustments often currently rely on estimating the classifier’s true and false positive rates (or their multi-class equivalents) from the training data and assumes that these rates are the same in the test population. This is similar to approaches used for transportability of clinical trial results, which use a weighted average of covariate conditional treatment effects obtained from the study sample to estimate the average treatment effect in a target population. (Westreich et al., 2017; Cole and Stuart, 2010). Thus, the assumption that the misclassification rates are the same in the training and test data can be viewed as a transportability assumption.

The conditional distribution of the predicted labels $a$ from a classification algorithm is given by

$$p(a \mid y) = \int_x p(a \mid x)p(x \mid y)dx.$$  (1)

Here, $p(a \mid x)$ is the prediction distribution from the algorithm, and is going to be same in the training and test sets for the same $x$. Hence, if we assume that $p_{tr}(x \mid y) = p_{\text{test}}(x \mid y)$, then we have $p_{tr}(a \mid y) = p_{\text{test}}(a \mid y)$ in (1). Hence, implicit in the transportability assumption $p_{tr}(a \mid y) = p_{\text{test}}(a \mid y)$ is that $p_{tr}(x \mid y) = p_{\text{test}}(x \mid y)$ (Pérez-Gállego et al., 2019), that is, we assume that the sensitivity and specificity of the classifier is same in
the training and test dataset. The marginal distributions of the outcomes $p_{tr}(y)$ and $p_{test}(y)$ are allowed to be different.

Dataset shift occurs when both $p_{tr}(y) \neq p_{test}(y)$ and $p_{tr}(x|y) \neq p_{test}(x|y)$ (Moreno-Torres et al., 2012). It is evident from (1) that under dataset shift, we will not generally have $p_{tr}(a|y) = p_{test}(a|y)$. This renders the assumptions of same sensitivity and specificity among the training and test sets used by most quantification methods invalid. An example of dataset shift is in the Population Health Metrics Research Consortium (PHMRC) gold standard dataset (Murray et al., 2011), which contains 168 reported symptoms and gold-standard underlying causes of death for adults in 4 countries. There are 21 total causes of death, that are then aggregated to 5 broader cause of death categories. Figure 1 shows the percentage of subjects within each country and cause of death that report each symptom. The $x$-axis is an enumeration of the entire list of symptoms $x$ and the $y$-axis plots $p(x|y)$ for each symptom $x$. With no dataset shift, we would expect the conditional response rates for each question within each cause of death to be similar for every country. However, as the country-specific lines are quite distinct in each sub-figure, it is clear that this assumption is violated. This leads to poor performance when using symptoms and cause of death labels from 3 countries to predict the cause of death distribution for the remaining country (McCormick et al., 2016).

When limited validation data with known labels is available from the test set, Datta et al. (2018) proposed population-level Bayesian Transfer Learning (BTL) – a quantification approach to address dataset shift which resourcefully combines this limited labeled data with the predicted labels for all test data. The labeled test data are used to estimate the misclassification rates $p(a|y)$ of the algorithm on the test set. Hence, BTL only uses the assumption that the misclassification rates are transportable from the labeled test data to the unlabeled test data. The marginal distribution of $y$ in the labeled test set is allowed to be different from that in the unlabeled test set. The large unlabeled data is used to estimate $p(a)$, which are then used to estimate $p(y)$. The two-estimation pieces are combined in a hierarchical model to offer Bayesian inference on $p(y)$.

BTL requires a single-class (categorical) prediction for each instance. Statistical classifiers are often probabilistic (McCullagh and Nelder, 1989; Murphy et al., 2006; Specht, 1990) producing a compositional prediction – the vector of prediction probabilities for every class. Hence, BTL categorizes these compositional predictions into categorical predictions by using the most probable category, and uses multinomial distributions to model the predicted labels. This categorization leads to information loss and Bella et al. (2010) showed that quantification using the class probability estimates can outperform such a practice.

In this manuscript, we generalize Bayesian quantification using limited labeled test data to use entire compositional prediction distributions from classifiers. Rather than positing a valid likelihood for compositional data, we use a Kullback-Liebler divergence loss equivalent to a Bayesian-style estimating equation for compositional data. The advantages of using this loss function over proper likelihoods for compositional data are many fold. The loss function is defined by a first moment (expectation) assumption and is robust to model misspecification. The loss function for the labeled data based on the conditional expectation is coherent with that for the unlabeled data based on the corresponding marginal expectation. Unlike Dirichlet
Figure 1: Percent of subjects with each of 168 reported symptoms within each of the 5 gold-standard underlying causes of death, by country.

higher-order distribution models for compositional data, the loss function approach allows 0’s and 1’s in the data. Also, importantly, this loss function remains the same no matter if one uses categorical single-class predictions or if one uses compositional probability predictions, subsuming the BTL model as a special case, when all data are categorical. The loss function harmonizes with conjugate priors for the parameters and a simple coarsening and rounding approximation leads to a fast and efficient Gibbs’ sampler.

Our second innovation concerns uncertainty in true labels in the labeled test set. This is not uncommon. For example, physicians may be uncertain in the final cause of death (McCormick et al., 2016), or labels may be produced by aggregating crowd sourced responses (Bragg et al., 2013). Existing quantification approaches do not allow for uncertainty in the true labeled test instances. We extend our approach to allow for probabilistic true labels. We use simple belief-based mixture modeling (Szczurek et al., 2010) to allow practitioners to specify the apriori class probabilities for instances in the labeled set.
Like BTL, we extend to an ensemble approach that can utilize predicted labels from multiple classifiers to produce an ensemble quantification that is robust to inclusion of poor classifiers in the group. We demonstrate how different choices of shrinkage priors ensures that, in the absence of labeled test data, i.e., when it is not possible to adjust for dataset shift, quantification from our method shrinks to different existing quantification methods like classify & count (CC), and adjusted classify & count (Forman 2005), or probabilistic average (PA) or adjusted probabilistic average (Bella et al, 2010). Hence, our approach provides a probabilistic inferential framework around each of these existing quantification approaches.

Finally, there is no supporting theory about the accuracy of Bayesian quantification under dataset shift in large sample settings. Bayesian updating of posteriors using loss-functions is termed generalized Gibbs updates or generalized belief updates. The seminal work of Bissiri et al (2016) explains the interpretation and statistical properties of such generalized posteriors. An immediate consequence of their work is that our loss-function, in an asymptotic sense, can be interpreted as a sum of two Bayes risks, one for the labeled data used to adjust for dataset shift and one for the unlabeled data to perform quantification. Going beyond this nice interpretation, we prove a theoretical guarantee about the asymptotic consistency of our quantification approach. The theory does not require full specification of a true model and only relies on the first-moment assumption being true for some parameter value. The theory easily accommodates the practical modifications used to implement the Gibbs sampler and extends to the case of multiple classifiers.

Because our model handles both single-class and probabilistic predictions from a classifier, allows uncertainty in true labels, uses generalized Gibbs updates, and subsumes existing quantification approaches as special cases, we term it Generalized Bayesian Quantification Learning (GBQL). The rest of the manuscript is organized as follows. The problem-setting and notation are introduced in Section 2 along with a review of existing quantification approaches. The method, various extensions, implementation, and posterior concentration results are presented in Section 3. We show the robustness of our method through simulations in Section 4 and in Section 5 we demonstrate its performance on the problem of deriving the cause-specific rates of child death using the PHMRC dataset.

2 Notation, assumptions, and review of quantification learning

We have N instances in our test set with predicted labels \( a = a(x) \) output from a pre-trained algorithm \( A \), but without the true labels \( y \). The instances are assumed to be randomly sampled from our population of interest and our interest lies in estimating the distribution of \( y \). We further assume availability of \( n \ll N \) instances from our population of interest with both true labels \( y \) and predicted labels \( a \). We do not assume that the training data for the algorithm is available, nor do we assume the knowledge of the covariates \( x \) for the test set, as long as \( a(x) \) is available to us. Because true labels are potentially expensive to obtain, \( n \) is typically much smaller than \( N \) (and potentially \( n \) can be zero at the beginning of a quantification project like burden of disease estimation in a country), so even if the covariates were available, the limited labeled data is
not sufficient for building a new classifier as the covariate vectors $x$ are typically high-dimensional.

We refer to the population from which we obtain unlabeled instances as $U$ and the sub-population from which we obtain labeled instances as $L$. Although $L$ is a subset of the same test population, we do not require the distribution of $y$ in $L$ to be representative of our whole population. This is because true labels for outcomes may only be available for a convenient sample. For example, true cause of death may only be diagnosed for individuals who die in settings such as a hospital, making it impossible to also randomly sample individuals with known labels from our population of interest. We only assume that the conditional distribution $p(x|y)$ is the same in the labeled and unlabeled instances. This transportability assumption for $p(x|y)$ between $L$ and $U$ is more likely to hold. For example, even if the marginal cause of death distributions are different for hospital and community deaths, given a cause $y$, the symptoms $x$ observed in the patient are likely to have similar distribution in both settings. The transportability assumption implies from (1) that $p(a|y)$ is also transportable between $L$ and $U$ as the classifier $p(\cdot|x)$ is learnt from training data and this distribution remains same given $x$ irrespective of the population $x$ is drawn from.

We let $y_r \in \{1, \ldots, C\}$ denote the true class (label) for each instance $r$ where $C$ is the the total number of categories. Our target of interest is $p = p_U(y) = (p_1, \ldots, p_C)'$, the distribution of the outcome $y$ in our population of interest $U$, i.e, $p_i = p(y_r = i | r \in U)$. An algorithm has been trained using labeled training data that produces a compositional score $a(x_r) = a_r = (a_{r1}, \ldots, a_{rC})$ for an instance $r$ with covariate $x_r$ such that $0 \leq a_r \leq 1$ and $\sum_{i=1}^{C} a_{ri} = 1$. These scores may be an actual estimate of $p(y_r = i|x_r)$, or simply a normalized degree of belief about whether $y_r = i|x_r$. If a classifier gives a (categorical) single predicted class $j$ for an instance, would have $a_{rj} = 1$ and $a_{rj'} = 0$ for $j' \neq j$. Note that because these scores are produced via the training data, these are only expected to be accurate in the $r \in$ training data, and not for $r \in U \cup L$.

The most simple quantification approach is called Classify & Count (CC) (Forman, 2005). CC requires that there is a single predicted class $j$ for each instance, so that $a_{rj} \in \{0,1\}$. The CC estimate of $p_i$ is simply

$$\hat{p}_i^{CC} = \frac{\sum_{r \in U} a_{ri}}{N}.$$  

An Adjusted Classify & Count (ACC) (Forman, 2005) method has been proposed to account for the fact that a classification algorithm is not expected to make perfect predictions, even for instances from the same population as the training data. ACC relies on cross-validation with the original training data to estimate the true positive and false positive rates ($tpr$ and $fpr$) of the classifier (for the base case of $C = 2$), and obtaining the following ACC estimate of $p_i$

$$\hat{p}_i^{ACC} = \frac{\hat{p}_i^{CC} - f_{pr}}{t_{pr} - f_{pr}}.$$  (2)

This method and its multi-class extensions (Hopkins and King, 2010) are inappropriate for quantification in the presence of dataset shift, as the $f_{pr}$ and $t_{pr}$ estimated from the training data will not be representative.
of the true \( fpr \) and \( tpr \) in the test population \( U \cup L \) \cite{Perez-Galleo2019}. Furthermore, \( \hat{p}_{i}^{ACC} \) can be outside of the restricted range of \([0,1]\), although \cite{Hopkins2010} correct for this using constrained optimization.

Bayesian Transfer Learning (BTL) \cite{Datta2018} also assumes \( a_{r} \)'s are categorical and first proposes a model-based version of Classify and Count as \( \sum_{r \in U} a_{r} \sim \text{Multinomial}(N, p_{CC}) \). Then adjustment for dataset shift follows from the simple observation that \( p_{CC} \) is actually \( p_{U}(a) \) and does not necessarily equal \( p = p_{U}(y) \). In fact, the two are related by the identity \( p_{CC} = M'p \) where \( M = (M_{ij} = (p(a_{r} = j \mid y_{r} = i, r \in U \cup L)) \) is the misclassification matrix of the classifier on the test population. This adjustment is conceptually the same as the one used by ACC and \cite{Hopkins2010}. Instead of using \( M = I \) (i.e., no adjustment as in CC) or \( M = M_{tr} \) (i.e., transportability of the conditional distributions between the training and test data as used in ACC), BTL estimates \( M \) using data from \( L \), i.e., only assumes transportability of the conditional distributions from the limited test subset \( L \) to all test data. BTL does not assume any transportability of the marginal distribution of \( y \) between \( L \) and \( U \). The joint Bayesian hierarchical framework is then specified as

\[
\sum_{r \in U} a_{r} \sim \text{Multinomial}(N, M'p) \\
a_{r} \mid y_{r} = i \sim \text{Multinomial}(1, M_{ir}) \text{ for } r \in L, i = 1, \ldots, C.,
\]

with \( M_{ir} \) denoting the \( i \)th row of \( M \). The advantages of the Bayesian frameworks are multifaceted. If the prior on \( p \) supported on the \( C \)-dimensional simplex (like a Dirichlet distribution), then so is the posterior. Hence, the posterior estimate of \( p \) is guaranteed to lie on the simplex, unlike ACC. BTL can exploit use of shrinkage priors for \( M \) to stabilize estimation when \( L \) is very small. The Bayesian setup also seamlessly allows for extensions like use of predictions from multiple classifiers, and allowing \( M \) and \( p \) to be a function of covariates, etc.

\cite{Bella2010} developed approaches to quantification similar to CC and ACC, but using probabilistic classifiers, i.e., \( a_{r} \) being a compositional outcome instead of a categorical outcome. The Probabilistic Average (PA) estimate of \( p_{i} \), \( \hat{p}_{i}^{PA} \), is obtained in the same manner as \( \hat{p}_{i}^{CC} \), but does not require \( a_{rj} \in \{0,1\} \). An adjusted version of the PA estimate (APA) uses probabilistic estimates of the \( tpr \) and \( fpr \) by taking the average estimated probability within each class; this is easily extended to 3 or more classes. However, like CC and ACC, they do not adjust for dataset shift. To our knowledge, there is no quantification method for dataset shift that utilizes the compositional predictions from probabilistic classifiers.

3 Method

3.1 Issues with Bayesian quantification using compositional labels

There are fundamental hurdles to extend the model in (3) when some or all \( a_{r} \) are compositional. The Dirichlet distribution and its generalizations \cite{Hijazi2009, Wong1998, Tung2018},
are the standard model for compositional data. However, there are several issues with specifying a Dirichlet model for $a_r$.

1. We allow the $a_r$ to take 0 and 1 values as the predictions can be categorical or compositional but with zeros as predicted probability for a subset of classes. Dirichlet distributions don’t support 0’s and 1’s, and would require forcing the $a_{rj}$’s to lie strictly in $(0, 1)$ using some arbitrary cutoff. Alternatively, one can use the zero-inflated Dirichlet distribution (Tang and Chen, 2018) to formally account for the presence of 0’s, which leads to a significant increase in the number of parameters.

A related point is that single-class classifiers can be viewed as a subclass of probabilistic classifiers, with the predicted distribution being degenerate. Hence, if using two classifiers, one with compositional predictions and one single-class predictions, use of the Dirichlet model for the former and a multinomial model for the latter is discordant.

2. The BTL approach (3) has a coherence property. The conditional model in the bottom-row $a_r| y = i \sim Multinomial(1, M_{i*})$ for $r \in U \cup L$ leads to the marginal model in the top row $a_r \sim \sum_{i=1}^{C} p_i Multinomial(1, M_{i*}) = Multinomial(1, M'p)$ for $r \in U$. Specifying $a_r| y = i$ as a Dirichlet distribution (or its variants), will endow $a_r$ with a mixture-Dirichlet marginal distribution which presents a computational challenge in posterior sampling.

3. Alternatively, one can enforce coherence in the conditional and marginal expectations by specifying models of the form $a_r| y = i \sim Dirichlet(\alpha_1 M_{i*})$ and $a_r \sim Dirichlet(\alpha_2 M'p)$. Such Dirichlet models are susceptible to model misspecification. While more complex models like generalized Dirichlet (Wong, 1998) can be used, increased model complexity comes with added computational burden.

4. The multinomial likelihood for $a_r$ nicely harmonizes with conjugate Dirichlet priors for the parameters $M$ and $p$ leading to an extremely efficient Gibbs sampler. Using a Dirichlet distribution based likelihood relinquishes this computational advantage as the priors no longer remain conjugate.

Finally, as an alternate to Dirichlet-based likelihoods, one can transform the data and use log-ratio models, which uses a multivariate normal or skew-normal to model the log-ratio coordinates of the compositional $a_r$ (Comas-Cufí et al., 2016). However, a transformation-free approach is generally more desirable. Also, a model on the transformed compositional $a_r$ will be discordant with the multinomial model for the categorical $a_r$. The transformations also generally do not allow for 0’s and 1’s.

### 3.2 Bayesian estimating equations for compositional data

Central to BTL’s estimation of population class probabilities (“quantification”)

$$p(y_r = i) = p_i, \ \forall r \in U$$

(4)
is the assumption of transportability of conditional distribution between $L$ and $U$, i.e.,

$$p(a_r | y_r = i) = M_{i*} \forall r \in U \cup L.$$  \hfill (5)

The distributional assumption (5) can also be viewed as a first-moment assumption

$$E(a_r | y_r = i) = M_{i*} \forall r \in U \cup L.$$  \hfill (6)

The two viewpoints are equivalent for categorical $a_r$ used in BTL, but (6) is more general as it is no longer restricted to categorical data. For compositional $a_r$, rather than specifying $p(a_r | y_r = i)$, we only make the general first moment assumption (6). This is similar to the first-moment assumption in the PA and APA approaches. The challenge is of course how to do valid Bayesian inference without a full model specification.

First focusing on labeled instances $r \in L$, we consider the following loss function to connect the parameter $M$ to our data $a_r, y$

$$\ell_L(M | \{a_r, y_r\}_{r \in L}) = \sum_{r \in L} D_{KL}(a_r || \sum_{i=1}^{C} M_{i*} I(y_r = i))$$  \hfill (7)

where $D_{KL}(p||q)$ is the Kullback–Leibler divergence (KLD) between two distributions $p$ and $q$. There are several reasons to choose the KLD loss functions. First, if (6) is true for some $M = M_0$, then

$$E_{M_0} \left( \frac{d\ell_L}{dM} \right) = 0.$$  \hfill (8)

To see this, observe that $d\ell_L/dM$ is the derivative of a multinomial likelihood. Hence, $E_{M_0}(d\ell_L/dM) = 0$ when $a_r$ are categorical. However, this derivative is only a linear function of $a_r$ and hence the expectation remains unchanged when we switch to compositional $a_r$ with the same conditional mean. Hence, the loss function $\ell_L$ leads to a set of unbiased estimating equations (Liang and Zeger [1986]) for compositional data.

The second advantage of using KLD is that, as $x \log x = 0$, it seamlessly accommodates instances 0’s and 1’s in $a_r$. Finally, minimizing (7) is equivalent to maximizing

$$\prod_{r \in L} \prod_{j=1}^{C} \left( \sum_{i} I(y_r = i) M_{ij} \right)^{a_{rj}}$$

which is the exact form of the multinomial quasi-likelihood (MQL). So, when $a_r$ are all categorical, this reduces to the likelihood from the second row of (3).

If only inference on $M$ was of interest, frequentist optimization on (7) or GEE using its derivative can be executed. Using the rich theory of estimating equations, the estimate $\hat{M}$ has been shown to be a consistent estimator for $M$ (Papke and Wooldridge [1996]; Mullahy [2015]), and such frequentist approaches have been
commonly used in the econometrics literature for regression with a compositional outcome.

However, the primary interest in quantification is in \( p \) and accurate estimation of the nuisance parameter \( M \) is only an important intermediate step. The unlabeled dataset \( U \) is the only one informing estimation of \( p \), and using (4) and (6), the marginal first-moment condition for \( a_r \) in \( U \) is given by:

\[
E[a_r] = E[E[a_r|y_r]] = \sum_i p_i E[a_r|y_r = i] = M'p, \forall r \in U. \tag{9}
\]

This harmonizes with the loss-function

\[
\ell_U(p, M|\{a_r\}_{r \in U}) = \sum_{r \in L} D_{KL}(a_r||M'p). \tag{10}
\]

The loss function \( \ell_U \) for the marginal distribution of the predicted labels is coherent with the loss-function \( \ell_L \) for their conditional distribution, as they are based off of coherent moment conditions (6) and (9). Assuming (4) and (6) holds for some true \( p_0 \) and \( M_0 \), following the same logic used in (8), we can show

\[
E_{M_0,p_0} \left( \frac{d\ell_U}{d(M,p)} \right) = 0, \tag{11}
\]

i.e., the derivative is once again an estimating equation. However, if we only considered \( \ell_U \) without bringing in \( \ell_L \), \( M \) and \( p \) cannot be identified. For example, \( \ell_U(M, p) = \ell_U(I, M'p) \). Hence, we will consider the joint loss-function \( \ell = \ell_L + \ell_U \) as adding \( \ell_L \) helps to identify \( M \) which in turns makes \( p \) identifiable.

Loss functions and estimating equations have traditionally been used in frequentist literature to yield inference robust to model misspecification. To conduct and justify Bayesian inference with loss functions, we invoke the fundamental results of Bissiri et al. (2016) who showed that for any reasonable choice of a loss-function \( \ell(\theta|\text{data}) \) and prior \( \Pi(\theta) \), generalized Gibbs posteriors of the form

\[
\Pi(\theta|\text{data}) \propto \exp (-\ell(\theta|\text{data})) \Pi(\theta)
\]

are valid posteriors provided the normalizing constant exists. This posterior is interpreted as the distribution \( \nu \) for \( \theta \) minimizing the loss function \( E_{\nu}(\ell(\theta|\text{data})) + D_{KL}(\nu, \Pi) \).

We will use the notation \( a^L \) and \( a^U \) to respectively denote the collections \( \{a_r\}_{r \in L} \) and \( \{a_r\}_{r \in U} \), and similarly for collections of the other variables. The two-loss functions \( \ell_L \) and \( \ell_U \) also have same functional form leading
to the generalized posterior:

\[
\Pi(p, M | a^U, a^L, y^L) \propto \exp \left( - \sum_{r \in U} D_{KL}(a_r || E[a_r]) - \sum_{r \in L} D_{KL}(a_r || E[a_r | y_r]) \right) \Pi(p, M) \\
\propto \exp \left( - \sum_{r \in U} \sum_{j=1}^C a_{rj} \log \frac{\sum_i p_i M_{ij}}{a_{rj}} - \sum_{r \in L} \sum_{j=1}^C a_{rj} \log \frac{\sum_{i=1}^C I(y_r = i) M_{ij}}{a_{rj}} \right) \Pi(p, M)
\]

If all \(a_r\) were categorical, this posterior is identical to the one from the BTL model \((3)\). However, using the estimating equations approach, we now have an unified framework for Bayesian quantification for both categorical, compositional or mixed-type \(a_r\) without having to specify the full models for the different data types.

### 3.3 Uncertainty in true labels

As stated in Section \([4]\) in many applications, there is uncertainty in some or all of the true labels in the labeled test set \(\mathcal{L}\). For example, a panel of physicians may fail to unanimously agree on a single cause of death, and only provide a subset of the list of causes from which they believe the individual was equally likely to die. In this Section, we modify the loss function \(\ell_L\) to incorporate uncertainty for class labels in \(\mathcal{L}\).

Following the belief based modeling framework of Szczurek et al. (2010), we let \(b_{ri}\) represent the apriori probability that instance \(r\) belongs to label \(i\). Then \(b_r\) is constrained such that \(0 \leq b_{ri} \leq 1\) and \(\sum_{i=1}^C b_{ri} = 1\).

Now for an instance \(r \in \mathcal{L}\) we no longer observe the \(y_r\)'s but observe the belief vector \(b_r\). Cases where the true label is identified with complete certainty can be subsumed by writing \(b_r = e_i\) when \(y_r = i\), \(e_i\) denoting the vector with 1 at the \(i^{th}\) component and zeros elsewhere. We can generalize the conditional first-moment condition \((6)\) to

\[
E[a_r | b_r] = E[E[a_r | y_r, b_r] | b_r] = E \left( \sum_i M_{i*} I(y_r = i) | b_r \right) = M' b_r
\]

and our loss function for \(\mathcal{L}\) becomes

\[
\ell_L(M | a^L, b^L) = \sum_{r \in \mathcal{L}} D_{KL}(a_r || M' b_r) = \sum_{r \in \mathcal{L}} \sum_{j=1}^C a_{rj} \log \left( \frac{\sum_{i=1}^C b_{ri} M_{ij}}{a_{rj}} \right)
\]

Of course, the loss for the unlabeled data remains the same, and Bayesian inference proceeds using the likelihood \(\ell_L + \ell_U\) with this generalized choice of \(\ell_L\).

Once again, appealing to the results from Bissiri et al. (2016), we can see that \(\nu = \Pi(p, M | a^U, a^L, b^L)\) is the
probability measure which, as \( n, N \to \infty \) and \( \frac{n}{N} \to \alpha \), minimizes the Bayes risk

\[
E_\nu \left[ \mathbb{E}_{r \in \mathcal{U}}[D_{KL}(a_r || M')] + \alpha \mathbb{E}_{r \in \mathcal{L}}[D_{KL}(a_r || M'b_r)] \right].
\]

### 3.4 Ensemble Quantification Incorporating Multiple Predictions

There may be \( k = 1, \ldots, K \) predictions for each instance corresponding to predictions from different classifiers. Datta et al. (2018) has already shown the advantage of incorporating multiple algorithms for quantification when only categorical predictions are available, and their ensemble quantification can easily be extended to compositional settings.

A fundamental observation for the ensemble approach is that each algorithm is expected to have their own sensitivities and specificities. Representing the \( k^{th} \) algorithm prediction for instance \( r \) as \( a^k_r \), the conditional first moment assumption (6) becomes

\[
E(a^k_r | y_r = i) = M^k_{si} \forall r \in \mathcal{U} \cup \mathcal{L},
\]

where \( M^k \) is the misclassification matrix of the \( k^{th} \) classifier on the test population. For the unlabeled data, we will now have the labels satisfying the marginal first moment condition \( E(a^k_r = M^k'p) \). Hence, each of the \( K \) predictions for the unlabeled test data \( \mathcal{U} \) informs about the same parameter \( p \) (which is our estimand) and we can conduct ensemble quantification by specifying the loss function as the sum of the losses for the individual algorithms:

\[
\sum_{k=1}^{K} \left[ \sum_{r \in \mathcal{U}} D_{KL}(a^k_r || M^{(k)}') p + \sum_{r \in \mathcal{L}} D_{KL}(a^k_r || M^{(k)}'b_r) \right]
\]

An advantage of this loss function is that it allows for combining information from probabilistic classifiers and non-probabilistic ones (like clinical classifiers for cause of deaths).

### 3.5 Gibbs Sampler using rounding and coarsening

We first outline the Gibbs sampler steps when only one predicted labels is available per instance. The sampler for ensemble quantification is detailed in the appendix. The generalized posterior distribution \( \nu \) is given by

\[
\nu \propto \left[ \prod_{r \in \mathcal{U}} \prod_{j=1}^C \left( \sum_i p_{ij} M_{ij} \right)^{a_{rj}} \prod_{r \in \mathcal{L}} \prod_{j=1}^C \left( \sum_i b_{rj} M_{ij} \right)^{a_{rj}} \right] \pi(p, M)
\]

When all \( a_r \) are categorical, the polynomial expansion of \( \left( \sum_i p_{ij} M_{ij} \right)^{a_{rj}} \) enabled an efficient latent variable Gibbs sampler in Datta et al. (2018). When \( a_{rj} \) are fractions, this advantage is lost as fractional polynomials
do not have such convenient expansions. Additionally, since we now allow uncertainty in the true labels, we also need to consider the extra fractional expansion terms \((\sum_i b_{ri}M_{ij})^{arj}\).

To enable fast and efficient sampling, we first switch from \(\nu\) to \(\nu_{\text{round}}\) where the probabilistic output \(a_{rj}\) is replaced by \([T a_{rj}]\) where \(T\) is an integer, and \([\cdot]\) denotes the ceiling of any real number. Consider now the following generative model:

\[
\begin{align*}
z_{rt}^{\text{ind}} & \sim \begin{cases} 
  \text{Multinomial}(1, p) & \text{if } r \in U \\
  \text{Multinomial}(1, b_r) & \text{if } r \in L
\end{cases} 
, \quad t = 1, \ldots, T_r = \sum_j [T a_{rj}]

d_{rt} | z_{rt} = i \sim \text{Multinomial}(1, M_{i*}), r \in L \cup U
\end{align*}
\]

The rounded generalized posterior \(\nu_{\text{round}}\) is then the proper Bayesian posterior using the likelihood \(p(d^U, d^L | b^L, M, p)\) for any realization of \(d_{rt}\)’s satisfying \(\sum_i I(d_{rt} = j) = [T a_{rj}]\). To obtain samples of \(p\) and \(M\) from \(\nu_{\text{round}}\), instead of using this marginalized likelihood, we can equivalently introduce \(z^L\), and \(z^U\) as latent variables and use the joint likelihood \(p(d^U, d^L, z^L, z^U | b^L, M, p)\). This joint likelihood decomposes nicely and will be conducive to a Gibbs sampler with standard Dirichlet priors on \(M\) and \(p\).

Next, since we artificially inflate sample size by an order of \(T\) by switching from \(a_r\) to \([Ta_r]\), instead of sampling from \(\nu_{\text{round}}\) we sample from the coarsened likelihood \(\nu_{\text{coarse}} \propto p(d^U, d^L | b^L, M, p)^{\frac{1}{T}} \pi(p, M)\).

Because \(p(d^U, d^L | b^L, M, p)\) is a proper likelihood, this implies that \(\nu\) can be expressed as a power posterior [Bhattacharya et al., 2019] [Ibrahim et al., 2015], and as \(p(d^U, d^L | b^L, M, p)\) is a mixture of categorical distributions, we can introduce latent variables into our Gibbs sampler by using the Conditional Coarsening Algorithm [Miller and Dunson, 2019] just like we would do for \(\nu_{\text{round}}\).

For outlining the Gibbs sampler steps, we use generic Dirichlet priors \(M \sim \text{Dirichlet}(V)\), i.e., \(M_{i*} \overset{\text{ind}}{\sim} \text{Dirichlet}(V_{i*})\), and \(p \sim \text{Dirichlet}(v)\) where \(V\) and \(v\) respectively are a matrix and a vector of positive hyperparameters. Specific choices with desirable shrinkage properties are discussed in Section 3.6. This gives the following Gibbs updates:
\textbf{Multinomial} \left(1, \frac{1}{\sum_{i \in U} M_{ij} p_i}, \ldots, \frac{1}{\sum_{i \in L} M_{ij} b_r i} \right), \quad r \in \mathcal{U}, \quad d_{rt} = j

\textbf{Multinomial} \left(1, \frac{1}{\sum_{i \in U} M_{ij} b_r i}, \ldots, \frac{1}{\sum_{i \in L} M_{ij} b_r i} \right), \quad r \in \mathcal{L}, \quad d_{rt} = j

\begin{align*}
M_{ij} &\sim \text{Dir} \left(\tilde{\nu}_i, \ldots, \tilde{\nu}_{ij} \right), \quad \tilde{\nu}_{ij} = \nu_{ij} + \frac{1}{T} \left( \sum_{r \in \mathcal{U}, \mathcal{L}} \sum_{t=1}^{T} (I(d_{rt} = j)I(z_{rt} = i)) \right) \\
p_{ij} &\sim \text{Dir} \left(\tilde{\nu}_i, \ldots, \tilde{\nu}_{ij} \right), \quad \tilde{\nu}_i = \nu_i + \frac{1}{T} \left( \sum_{r \in \mathcal{U}} \sum_{t=1}^{T} I(z_{rt} = i) \right)
\end{align*}

If there are hyper-parameters \( \gamma \) in \( V \) and \( v \) that need to be assigned a prior, they can be sampled using a Metropolis-Hastings step. We note that the full conditional distributions for the \( z_{rt} | d_{rt} = j \) for \( r \in \mathcal{U} \) are identical, which enables them to be jointly sampled. Furthermore, the \( z_{rt} \) for \( r \in \mathcal{L} \) do not need to be updated if there is a \( i \) such that \( b_{ri} = 1 \). We find that setting \( T = 100 \) works well in practice, and that there is little information to be gained by finer coarsening.

### 3.6 Shrinkage towards default quantification methods

We now discuss how existing quantification approaches are special cases of GBQL with specific choices of degenerate priors for \( M \), and how we leverage this knowledge to construct shrinkage priors in data-scarce settings.

Quantification projects like burden of disease estimation using nationwide surveys are often multi-year endeavors, and at the initial stages of such projects, \( \mathcal{L} \), consisting of hospital deaths with clinically diagnosed causes, can be very small. With very limited labeled data, estimating both \( M \) and \( p \) precisely with vague priors is ill-advised as \( M \) involves \( C(C-1) \) parameters. Hence, it is important to carefully choose priors that stabilize estimation of \( M \).

We first make the following observations for the scenario where \( n = 0 \), i.e., when there is no labeled test set to estimate dataset shift. Consider a sequence \( \{\Pi_u(M) \mid u = 1, 2, \ldots\} \) of priors for \( M \) such that \( \Pi_u \) converges in distribution to the degenerate prior at some pre-fixed transition matrix \( M^{pr} \). Then the posterior \( \nu_u \) using the prior \( \Pi(p)\Pi_u(M) \) converges in distribution to

\[
\lim_{u \to \infty} \nu_u(p) \propto \exp \left( -\sum_{r \in \mathcal{U}} D_{KL}(a_r || M^{pr} p) \right) \Pi(p)
\]

If \( M^{pr} = I \), then for any prior choice of \( p \), \( \lim_{u \to \infty} \nu_u(p) \propto \text{Dirichlet}(\sum_{r \in \mathcal{U}} a_r)\Pi(p) \). In particular, if \( \Pi(p) = \text{Dirichlet}(0) \) or as \( N \to \infty \), then \( \lim_{u \to \infty} \nu_u(p) = \text{Dirichlet}(\sum_{r \in \mathcal{U}} a_r) \). For categorical \( a_r \), this result was proved in [Datta et al. (2018)](Datta2018), and shows that \( E_{\lim_u \nu_u(p)} = p^{CC} \), i.e., using priors \( \Pi_u(M) \) shrinking towards the degenerate prior at \( I \), inference from GBQL becomes identical to inference from Classify and
Count \cite{Forman:2005} when there is no labeled dataset. Analogously, for the same settings, when \( a_r \) are compositional, posterior mean from GBQL becomes identical to Probabilistic Average \cite{Bella:2010}. Extending, the argument to the settings with multiple predictions, it is straightforward to see that
\[
E_{\lim_{\nu_u \to \infty}}(p) = 1/K \sum_{k=1}^{K} p^k PA,
\]
i.e., the posterior mean from our ensemble classifier coincides with the average of the PA estimates for the \( K \) classifiers.

Alternatively, if the misclassification matrix \( M^{tr} \) for the training data is available and can be trusted for test data, one can use \( M^{pr} = M^{tr} \). Then the posterior \( \lim_{\nu_u \to \infty} \nu_u(p) \) coincides with the implicit likelihood in Adjusted Classify and Count (for categorical \( a_r \)) and in Adjusted Probabilistic Average (for compositional \( a_r \)). In fact, using \( \Pi(M) \approx \delta(M = M^{tr}) \) in GBQL is a better implementation of ACC or APA, as the proper posteriors ensure that the estimate (posterior mode or mean) of \( p \) is guaranteed to be a vector of probabilities lying in \([0, 1]\). This is not assured in their current implementation based on the direct correction (2).

Hence, in absence of local labeled set, a prior for \( M \) concentrated around \( I \) or \( M^{tr} \), makes estimates from GBQL nearly coincide with these existing methods (Figure 2). GBQL also provides a probabilistic framework around these existing quantification approaches, and using the full posterior samples of \( p \), one can now pursue any inferential quest for each of these approaches beyond just the point estimation. The classes of shrinkage priors for \( M \) are easy to construct. For example, the priors \( M_i \sim \text{Dirichlet}(\gamma_{ui}(M_{i}^{pr} + \epsilon_{u} 1)) \) concentrates around \( \delta(M = M^{pr}) \) if either \( \epsilon_{u} \to 0 \) or \( \gamma_{ui} \to \infty \).

When we will have small amounts of labeled data, using these shrinkage priors will make a bias-variance tradeoff yielding estimates with higher precision. The benefits of such shrinkage priors over non-informative priors have been demonstrated in \cite{Datta:2018} in such settings. Finally as more and more labeled data is collected, in the next section we show that any reasonable choice of prior (including all these shrinkage priors) leads to desirable asymptotic concentration of the posterior.

### 3.7 Theory

Our quantification approach is grounded in the only assumption that for both \( L \) and \( U \), the conditional first moment of \( a_r \mid y_r \) are correctly specified as in \cite{Kessler:2015}. Throughout we do not make any other assumptions about higher moments or full distributions. \cite{Kessler:2015} have used a similar first moment assumption to develop a Gibbs sampling approach for compositional regression. However, their approach only incorporates the rounded likelihood for the psuedo-data \( d_r \), and does not coarsen. Rounding inflates the sample size by a factor of \( T \) resulting in underestimation of the posterior variance and the coarsening is needed to adjust for this. We will show that the coarsening adjustment by this factor of \( T \) ensures asymptotic equivalence of the rounded and coarsened posterior \( \nu_{coarse} \) with the original posterior \( \nu \). \cite{Yuan:2007} also used a similar Gibbs sampler in the context of early-phase clinical trials with multiple toxicity grades. However, both \cite{Yuan:2007} and \cite{Kessler:2015} did not provide any theory backing the use of a Gibbs sampler based on a loss-function instead of a proper likelihood or justified the
approximations used in the Gibbs sampler. We have already justified using the first-moment assumption in a Bayesian framework, by appealing to the results of Bissiri et al. (2016). In this section we also establish posterior consistency of both \( \nu \) and the rounded and coarsened posterior \( \nu_{\text{coarse}} \) used in the Gibbs sampler.

We develop the theory for the general case where the true labels in \( \mathcal{L} \) are observed with uncertainty \( b_r \) which subsumes the case with exact labels \( y_r \). We will use \( \tilde{M} \) and \( \tilde{p} \) to denote the free parameters in \( M \) and \( p \) respectively, i.e., \( \tilde{M} \) excludes the last column of \( M \), \( \tilde{p} \) excludes the last element of \( p \). \( M \) and \( p \) are bijective functions of \( \tilde{M} \) and \( \tilde{p} \) respectively, so we will use them interchangeably. Let \( \theta = (\tilde{M}, \tilde{p}) \), then \( \theta \) is supported on the compact set \( \Theta = S_{d-1}^C \otimes S_{C-1} \) where \( S_d = \{ x \in \mathbb{R}^d \mid x_i \geq 0, 1'x \leq 1 \} \). Switching to \( \tilde{M} \) and \( \tilde{p} \) ensures

Figure 2: GBQL includes and extends the common quantification methods through different classifier outputs and choices of priors for \( M \). Red lines indicate the settings where GBQL extends current methods, while black lines indicate where GBQL subsumes existing methods.
that the parameter space $\Theta$ has a non-empty interior. The generalized posterior from Section 3.3 is given by:

$$
\nu_N(\theta) = \Pi(p, M| a^i, a^C, b^C) \propto \exp \left( - \sum_{r \in \ell} D_{KL}(a_r||M^r) - \sum_{r \in \ell} D_{KL}(a_r||M^r) \right) \Pi(p, M).
$$

(14)

Let $p^0$ and $M^0$ denotes the true values and $\theta^0 = (\overline{M}^0, \overline{p}^0)$ be an interior point in $\Theta$. We first state our assumptions, for the theory:

1. The matrix $B_j$, formed by column-stacking $b_i$’s for $r \in \ell$ such that $a_{rj} > 0$, has full row rank.
2. $M^0$ is non-singular.

**Theorem 1.** Let $B_j(\theta^0)$ be the Euclidean ball of radius $\epsilon$ around $\theta^0$, and $\Pi(p, M)$ be any prior which gives positive support to $B_j(\theta^0)$ for any $\epsilon > 0$. Then, under assumptions 1-2, as $N, n \to \infty$ and $n/N$ to some limit, for any $\epsilon > 0$, $P_{\nu_N}(B_j(\theta^0)) \to 1$.

While the formal proof is provided in the appendix, we briefly outline the ideas used here which will also help to contextualize the assumptions. We can write $\nu_N(\theta) \propto \exp(-\ell_{\ell,n}(\overline{M}) - \ell_{U,N}(\theta))\Pi(\overline{p}, \overline{M})$ where the subscripts $n$ and $N$ are added to indicate dependence of $\ell_{\ell,n}$, $\ell_{U}$ and $\nu$ on the sample size. Recently, Miller (2019) has provided very general and useful conditions for establishing asymptotic concentrations of generalized posteriors of the form $\exp(-N f_N(\theta))\Pi(\theta)$. One of the general tricks is to show that the functions $f_N$ converge point-wise to some function $f$, and that $f_N$’s and $f$ are convex. These conditions are sufficient for the generalized posterior to concentrate around $\theta^0$, the minimizer of $f$. In our case, $f_N = (\ell_{\ell,n} + \ell_{U,n})/N$ converges point-wise to $f = \alpha E_L(D_{KL}(a||M^r b)) + E_U(D_{KL}(a||M^r p))$ where $\alpha = \lim n/N$. However, neither $f_N$’s nor $f$ is convex because of the $M^r p$ term, ruling out direct application of this result.

We first focus just on $\ell_{\ell,n}/n$ and establish the result

**Lemma 1.** If Assumption 1 holds, then for any $\epsilon > 0$ the generalized posterior $\nu_{\ell,n}(\overline{M}) \propto \exp(-\ell_{\ell,n})\Pi(\overline{M})$ satisfies,

(a) $P_{\nu_{\ell,n}(\overline{M})}(B_j(\overline{M}^0)) \to 1$.

(b) $\lim \inf_{n} \inf_{\overline{M} \notin B_j(\overline{M}^0)} \ell_{\ell,n}/n > E_L(D_{KL}(a||M^r b))$.

Assumption 1 is needed to ensure that the loss-functions $\ell_{\ell,n}$ are convex. To interpret Assumption 1, we consider the special case where we observe the true labels $y$, and the predicted labels $a$ are categorical. Then this condition reduces to the statement that for every $(i, j)$ pair, there are cases in $\ell$ for whom the true class is $i$ and the predicted class is $j$. This is of course necessary to estimate the misclassification rate $M_{ij}$. Thus, Assumption 1 can be interpreted as a positivity assumption requiring that the limited labeled test set has data enough correctly estimate the sensitivities and specificities of the classifier for all class-pairs.

Lemma 1(a) is important on its own right as it establishes a consistency result for model-free Bayesian estimating equations for compositional regression. It states that when only loss $\ell_{\ell,n}$ is considered, the coefficients $M$ for the regression equation (6) is consistently estimated by generalized posteriors from KLD
loss function. We do not even need to actually observe the true labels \( y \) as observing the beliefs \( b \) suffices.

For our quantification problem, however, Lemma 1(b) is more relevant. As our \( f_N \)'s are not convex, an alternative sufficient condition to establish posterior concentration is that for large enough \( N \), the value of \( f_N \) outside any neighborhood around the true \( \theta^0 \) is strictly greater than \( f(\theta^0) \) (Miller, 2019). Lemma 1(b) states that outside of any neighborhood around the true value \( \mathbf{M}^0 \), the empirical loss-function \( \ell_{\mathcal{L},n} \) has higher value than the limiting loss-function \( E_{\mathcal{L}}(D_{KL}(\mathbf{a}||\mathbf{M}^0b)) \). A complementary result to Lemma 1(b) is that Lemma 2. \( \lim_{N \to \infty} \inf_{\theta \in \Theta} \ell_{\mathcal{U},N}(\mathbf{M},p) \) exists and equals \( E_{\mathcal{U}}(D_{KL}(\mathbf{a}||\mathbf{M}^0p)) \).

Lemma 2 states that the infimum value of \( \ell_{\mathcal{U},N}(\mathbf{M},p) \) over the entire space \( \Theta \) equals in the limit of \( N \to \infty \) to the limiting loss-function \( E_{\mathcal{U}}(D_{KL}(\mathbf{a}||\mathbf{M}^0p)) \) evaluated at true \( \theta^0 \). Combining, Lemmas 1(b) and 2, we have that for any region \( R \) of \( \Theta \), \( f_N(\theta) \) is greater than \( f(\theta^0) \) unless \( R \) lies in an infinitesimally small neighborhood around \( \mathbf{M}^0 \). Thus, use of the local labeled set \( \mathcal{L} \) via the loss function \( \ell_{\mathcal{L},n} \) helps to identify \( \mathbf{M} \), as the posterior is guaranteed to concentrate around \( \mathbf{M}^0 \). As \( \mathbf{M} \) concentrates around \( \mathbf{M}^0 \), the loss \( \ell_{\mathcal{U},N}(\mathbf{M},p) \) becomes capable of identifying \( p \). A sufficient condition for this is that \( \ell_{\mathcal{U},N}(\mathbf{M}^0,p) \) is a convex function of \( p \). Assumption 2 ensures this convexity. It is a separability assumption necessary for quantification as if there exists two probability vectors \( p^0 \) and \( p^1 \) such that \( \mathbf{M}^0p^0 = \mathbf{M}^0p^1 \) then it will be impossible to identify \( p \) based on predicted labels. This separability, or identifiability, assumption has long been discussed in the finite mixture model literature (Teicher, 1963; Yakowitz and Spragins, 1968), but has not been explicitly discussed for methods which rely on conditional first moments of classifier output for quantification.

Theorem 1 guarantees posterior concentration when using the actual generalized posterior \( \nu \). However, our Gibbs sampler relies on rounding and coarsening \( \nu \) using an integer factor \( T \). The following result connects the theory to the practical implementation.

Corollary 1. Let \( \nu_{\text{coarse},N} \) denote the rounded and coarsened generalized posterior using a factor \( T_N \) with \( T_N \to \infty \). Then, under the conditions for Theorem 1 we have \( P_{\nu_{\text{coarse},N}(\theta)}(B_\epsilon(\theta^0)) \to 1 \).

Corollary 1 makes it evident that not only the coarsening step is important, the coarsening and rounding factor \( T_N \) needs to increase with increase of sample size.

Finally, it is trivial to extend the posterior concentration results for the ensemble quantification.

Corollary 2. If \( K \) predictions are available for each label, and assumptions 1 and 2 are satisfied for each of the \( K \) prediction algorithms, then with \( \theta = (\mathbf{M}^{(1)}, \ldots, \mathbf{M}^{(K)}, \bar{p}) \) we have \( P_{\nu_{\text{coarse},N}(\theta)}(B_\epsilon(\theta^0)) \to 1 \).

4 Simulations

We conduct multiple simulation studies to assess

1. accuracy of GBQL in estimating \( p \) in the presence of moderate amounts of labeled data
2. comparison of our estimating equations based approach with Dirichlet model-based approach using
different data generating mechanisms

3. computation efficiency compared to Dirichlet model based approaches

4. estimation accuracy when there is uncertainty for some true labels in $L$.

To mimic the motivating verbal autopsy application, we used $N = 1000$, $n = 300$, $C = 5$, $p_L = E_L(y_r) = (\frac{1}{5}, \ldots, \frac{1}{5})$, and the following four different values of $p$ representing each of the four countries in the PHMRC dataset (Section 1)

$$p_1 = (.20, .19, .27, .27, .07)$$

$$p_2 = (.11, .11, .40, .29, .09)$$

$$p_3 = (.09, .18, .52, .19, .02)$$

$$p_4 = (.13, .30, .35, .19, .03)$$

We generated true labels

$$y_r|p, p_L \sim \begin{cases} 
\text{Multinomial}(1, p), & r \in \mathcal{U} \\
\text{Multinomial}(1, p_L), & r \in \mathcal{L}
\end{cases}$$

For the first analyses, we allow for full knowledge of these labels for $r \in \mathcal{L}$, which means that $b_r|y_r = i$ equals $e_i$ for $r \in \mathcal{L}$. We then simulated outputs $a_r|y_r$ directly from a model, so that we know the true data generating mechanism of the dataset shift. We let

$$M = \begin{bmatrix} 
0.65 & 0.35 & 0 & 0 & 0 \\
0 & 0.35 & 0.65 & 0 & 0 \\
0.1 & 0.1 & 0.6 & 0.1 & 0.1 \\
0 & 0 & 0 & 0.8 & 0.2 \\
0 & 0.4 & 0 & 0 & 0.6
\end{bmatrix}$$

and use two data generating mechanisms for $a_r|y_r$. The first mechanism corresponds to a zero-inflated Dirichlet mixture model:

$$a_{rj}^*|y_r = i, M_{ij} \sim \begin{cases} 
0, \text{ if } M_{ij} = 0 \\
\text{Gamma}(5M_{ij}, 1), \text{ else}
\end{cases} \quad j = 1, \ldots, C$$

$$a_{rj} = \frac{a_{rj}^*}{\sum_{k=1}^C a_{rk}^*}.$$
The second data generating mechanism introduced overdispersion in the data:

\[
\tau_r \sim 0.5 \cdot \text{Uniform}(1, 1) + 0.5 \cdot \text{Uniform}(10, 20)
\]

\[
a_{rj}^* | y_r = i, M_{i*} \sim \begin{cases} 
0, & \text{if } M_{ij} = 0 \\
\text{Gamma}(\tau_r \cdot M_{ij}, 1), & \text{else}
\end{cases}
\]

\[
a_{rj} = \frac{a_{rj}^*}{\sum_{k=1}^C a_{rk}^*}.
\]

Instances for which \(\tau_r \leq 1\) will have responses \(a_{rj}\) close to 0 and 1, while instances with larger values of \(\tau_r\) will have \(a_{rj}\) clustered closer to the non-zero entries of \(M\).

We then compare our method’s estimates of \(p\) with estimates from following standard Bayesian Dirichlet mixture model which assumes the first data generating mechanism as truth.

\[
y_r | p \sim \text{Multinomial}(1, p)
\]

\[
a_r | y_r = i \sim \text{Dirichlet}(\tau_i \cdot M_{i*})
\]

\[
\tau_i \sim \text{Normal}(0, 25)
\]

For both the Dirichlet model and the GBQL model, we used Dirichlet priors for \(M\) shrinking towards \(I\), and uninformative Dirichlet prior for \(p\).

Since the Dirichlet distribution does not support zeros, for running the Dirichlet model, 0 values were replaced with \(\epsilon = .001\) and each \(a_r\) was re-normalized. Posterior sampling for this model was performed using RStan Version 2.19.2 (Stan Development Team [2019]). Note that this model then becomes misspecified for the second true data generating mechanism. For both models, we ran three chains each with a total of 6,000 draws and a burn-in of 1,000 draws. We used the posterior mean of \(p\) as \(\hat{p}\).

To compare estimates of \(p\), we use a chance corrected version of the normalized absolute accuracy (NAA) (Gao and Sebastiani 2016) for estimating a compositional vector. NAA is defined as

\[
1 - \frac{\sum_{i=1}^C |p_i - \hat{p}_i|}{2(1 - \min_i \{p_i\})}.
\]

To represent random guessing of \(p\) with a score of 0, and perfect estimation of \(p\) with a score of 1, we follow Flaxman et. al (2015) and use the Chance Corrected NAA

\[
CCNAA = (\text{NAA} - .632)/(1 - .632).
\]

We repeat our simulations 500 times for each choice of \(p\) and show the average CCNAA across this simulations in Figure 2. For case 1 (left panel) when the likelihood is correctly specified for the Dirichlet model, both methods produce accurate estimates of \(p\) and have approximately the same CCNAA. When we introduce
overdispersion to the distribution of the $a_r | y_r = i$ (right panel), we see that the performance the GBQL model is hardly affected, and substantially outperforms the now misspecified Dirichlet model in all cases.

![Figure 3: Columns shows results for the two different data generating mechanisms, while each color represents each of the four true values of $p$. The GBQL model produces high values of CCNAA for each of the scenarios, while assuming a Dirichlet mixture model likelihood only produces acceptable estimates of $p$ when the likelihood correctly identifies the true data generating mechanism.](image)

When we investigated the Stan output for the Dirichlet models, many of the chains failed to converge when the likelihood was misspecified (Table 1). Furthermore, on average the Stan model took nearly 200 times longer to run than the GBQL method (Table 1). Thus, GBQL accurately estimates $p$, removes the need to correctly specify the likelihood, is fast, and does not require fine-tuning for the posterior samples to converge.

| Value for $p$ | Average $\hat{R}$ GBQL | Average $\hat{R}$ Dirichlet | Average Runtime (minutes) GBQL | Average Runtime (minutes) Dirichlet |
|---------------|-------------------------|-----------------------------|-------------------------------|----------------------------------|
| $p_1$         | 1.03                    | 3.32                        | 0.15                          | 29.79                            |
| $p_2$         | 1.02                    | 3.43                        | 0.16                          | 29.70                            |
| $p_3$         | 1.03                    | 3.12                        | 0.16                          | 28.84                            |
| $p_4$         | 1.03                    | 3.46                        | 0.15                          | 29.88                            |

Table 1: Average $\hat{R}$, as a measure of posterior sampling convergence, and runtime in minute for each value of $p$ was computed for when there is overdispersion in the data generating mechanism.

We now examine the behavior of the GBQL model in the case of uncertain labels. To induce this uncertainty, we generate the compositional $b_r$ from the following overdispersed Dirichlet distribution

$$
\tau_r \sim .5 \cdot \text{Uniform}(1, 1) + .5 \cdot \text{Uniform}(10, 20)
$$

$$
b_r \sim \begin{cases} 
\text{Dirichlet}(\tau, p), & r \in \mathcal{U} \\
\text{Dirichlet}(\tau, p_L), & r \in \mathcal{L}
\end{cases}
$$
and generate \( y_{ir} | \mathbf{b}_r \sim Multinomial(1, \mathbf{b}_r) \). The data generating process for the \( \mathbf{a}_r \) is the same as in the simulations with known labels. The compositional \( \mathbf{b}_r \) are used as the uncertain labels for \( r \in \mathcal{L} \). Figure 4 plots the average CCNAA from GBQL with known labels \( y \) against CCNAA of GBQL with unknown labels \( \mathbf{b} \) for each value of \( \mathbf{p} \) and data generating mechanism. It can be seen that introducing uncertainty in the labels results in slightly lower (upto 10%) CCNAA values indicating the small price we pay for the added uncertainty.

5 PHMRC Dataset Analysis

We now apply GBQL to the PHMRC dataset introduced in Section 1. The number of observations within India, Mexico, Philippines, and Tanzania are 2973, 1586, 1259, and 2023, respectively. To address country-specific dataset shift, for each country, we used the three remaining countries as training data for four methods commonly used for cause of death predictions: InterVA (Byass et al., 2012), InSilicoVA (McCormick et al., 2016), NBC (Miasnikof et al., 2015), and Tariff (Serina et al., 2015). The first three methods are probabilistic, while Tariff produces a score for each cause that needed to be normalized to be in \([0, 1]\). Model training was done using the openVA package version 1.0.8 (Li et al., 2019). We considered both compositional predictions (for Tariff, this was the normalized score) and classifications (single-class categorical predictions based on the most likely cause of death for an individual per each algorithm). For GBQL in the test country, we then sampled labeled data \( \mathcal{L} \) of varying sizes (n=25, 100, 200, 400) to investigate the effect of increasing the number of known labels. Sampling was performed such that \( \mathbf{p}_\mathcal{L} = (\frac{1}{5}, \ldots, \frac{1}{5}) \), as in Section 4. For comparisons,
we obtained estimates using the Probabilistic Average (PA, Bella et al., 2010) method for compositional predictions, which should align with the GBQL estimate for $n = 0$ (Section 3.6) for our choice of priors, as well as estimates using the Adjusted PA method. We repeated this 500 times for each size of $n$. Results for the average CCNAA when using compositional predictions are shown in Figure 5a.

When no labeled instances are available, we see that the APA method performs worse than the PA method across almost all countries and algorithms, demonstrating why it is not appropriate to estimate $\mathbf{M}$ using the training data in the presence of dataset shift. We see that obtaining $n = 25$ labeled instances (an average of only 5 labeled deaths per class) does not effectuate any improvement in the performance over not having any labeled test data ($n = 0$). However, increasing this to 100 labels (an average of 20 labeled deaths per class) leads to large increase in CCNAA indicating substantial improvement in estimation of $\mathbf{p}$ across all countries and algorithms. As there are 168 covariates used for building these classifiers, using just 100 observations to build a reliable classifier would be difficult, if not impossible. Quantification accuracy continues to increase with a larger number of labeled observations across all countries and algorithms, although the extent of this improvement is quite variable. Figure 5b compares the CCNAA for GBQL using compositional predictions versus GBQL using single-class categorical predictions. We see that using the original compositional scores offers improvement over categorization for all algorithms except Tariff for Philippines and Tanzania. The exception for Tariff is probably due to the fact that Tariff does not produce truly compositional predictions, but only scores which were normalized to artificially create the compositional scores.

Figure 5a shows that classifier performance varies widely across settings. We now look at the performance of our ensemble method which uses predictions from all four algorithms. Figure 6 shows the CCNAA for the ensemble method and the individual algorithms for different numbers of labeled observations and each country. With only 25 labeled observations, the ensemble CCNAA is approximately an average of the CCNAA for each of the other algorithms, which is what we would expect, as for $n = 0$ it is exactly the average as discussed in Section 3.6. With more labeled observations, the ensemble begins to either outperform all of the methods, or has CCNAA very close to that of the top performing method. Importantly, the ensemble method significantly outperforms the worst method for all combinations of country, output format and numbers of labeled observations, showing that including multiple algorithms and using the ensemble quantification protects against inadvertently selecting the worst algorithm.

Finally, to illustrate the efficacy of GBQL even when true labels are observed with uncertainty, we create a toy dataset by randomly pairing individuals within a country in the PHMRC data. To introduce label uncertainty into the analysis, for a pair of individuals, $r1$ and $r2$, we let

$$b_{r1i} = b_{r2i} = \frac{1}{2}(I(y_{r1i} = 1) + I(y_{r2i} = 1)),$$

By using two individuals each with a single (but possibly different) true label, we create two individuals each with uncertain observed labels in such a way that the total number of individuals with a given cause
(a) Average CCNAA for increasing numbers of labeled observations across all countries in the PHMRC dataset for four common VA algorithms. Average CCNAA for GBQL using compositional predictions is shown in green. We also compare the performance of GBQL to the PA (blue) and APA (red) methods.

(b) Comparison of CCNAA between GBQL using compositional predictions versus single-class/categorical predictions. Each point represents a different value of $n$, with the black line representing the identity line.

Figure 5: PHMRC data analysis using different quantification methods.
Figure 6: CCNAA comparing the ensemble GBQL (red) with the 4 individual GBQL algorithms across countries for both classification predictions and probalistic predictions.

Figure 7: Comparison of CCNAA when using known labels versus labels with uncertainty. Each point represents a different value of $n$, with the black line representing the identity line.

remains same in this new dataset as that in the actual PHMRC dataset. In other words, the data generation satisfies the assumption that $p(y_r = i | b_r) = b_{ri}$. We then used these beliefs instead of the true labels as input for our method. Figure 7 compares the CCNAA for the individual methods across each value of $n$ for compositional predictions when using the known labels versus representing uncertainty in the labels through beliefs. Generally, the performance of GBQL is similar for both types of inputs with the CCNAA when labels are observed with uncertainty generally doing slightly worse as in Section 4.

6 Discussion

Quantification is an important and challenging problem that has only recently gained the attention it deserves. There are important limitations of the commonly used methods; CC (Forman 2005), ACC (Forman 2005),
PA (Bella et al., 2010), and APA (Bella et al., 2010) as they do not use a probabilistic framework and only use training data, and therefore do not account for dataset shift. In absence of local labeled data, GBQL with specific choices of priors yields model-based analogs for each of these methods and provides a probabilistic framework around these approaches to conduct inference beyond point-estimation. In presence of local test data GBQL leverages it and substantially improves quantification over these previous approaches. In such settings, GBQL extends BTL (Datta et al., 2018) which does not allow uncertainty in either the predicted or the true labels. In summary, GBQL generalizes all these methods, allowing for both categorical and compositional classifier output, incorporation of training data (through priors) and labeled test data, and uncertain knowledge of labeled data classes.

Appealing to the fundamental results of Bissiri et al. (2016) on generalized posteriors, our paper proposes novel ideas about model-free Bayesian inference on compositional data that will find applications beyond the quantification problem. The Bayesian estimating equations and the KLD loss functions rely only on a simple first-moment assumption for compositional data that circumvents the need for full model specification even in a Bayesian setting. The KLD loss also allows 0’s and 1’s in the compositions thereby ensuring unified treatment of both compositional, sparse-compositional and categorical data. In addition, the loss function approach easily extends to harmonize output from multiple classifiers, leading to a unified ensemble method which is a pragmatic solution guarding against inadvertent inclusion of a poorly performing classifier in the pool of algorithms. The Bayesian paradigm enables use of shrinkage priors to inform the estimation of $M$ and $p$ when limited labeled data from the test set is available. The GBQL generalized Gibbs posterior exhibits posterior consistency, as does the coarsened posterior used for extremely fast posterior sampling. To our knowledge, these are the first results for consistency of Bayesian quantification in presence of local labeled test data. Finally, extensive simulations and PHMRC data analysis show that the GBQL model is robust to model misspecification, and uncertainty in true labels, and significantly improves quantification in the presence of dataset shift.

Currently the GBQL method gives equal weight to all instances in $U$ and $L$. For ongoing quantification projects, $p_{test}(x, y)$ may not be stable over time, and equally weighting instances collected early during the project may lead to inaccurate estimates of the current value for $p$. A potential solution could incorporate power priors (Ibrahim et al., 2015) for earlier observations, although we leave this for future research.

We are also pursuing further research on general moment-based Bayesian methods for compositional data that builds on our application of the results from Bissiri et al. (2016). Given that our loss function is the one used in MQL based regression approaches, this manuscript justifies using priors on the regression parameters of interest, and updating these beliefs with a MCMC based method. In addition, our method could generally be used for semi-supervised mixture modeling of compositional observations. Important future contributions would be instance level class predictions and incorporation of higher moments through our loss function approach.
A Appendix

A.1 Gibbs sampler for ensemble quantification

\[ z_{rt}^{(k)} \mid \sim \begin{cases} \text{Mult} \left( 1, \frac{1}{\sum_{i=1}^{M(k)} p_i}, \ldots, M_{Cj}^{(k)} p_C \right), & r \in U, \; d_{rt} = j \\ \text{Mult} \left( 1, \frac{1}{\sum_{i=1}^{M(k)} b_i}, \ldots, M(C)^{(k)} b_C \right), & r \in L, \; d_{rt} = j \end{cases} \]

\[ M_i^{(k)} \mid \sim \text{Dir} \left( \tilde{V}_{i1}^{(k)}, \ldots, \tilde{V}_{ij}^{(k)} \right), \; \tilde{V}_{ij} = V + \frac{1}{T} \left( \sum_{r \in U, L} \sum_{t=1}^{T} I(d_{rt} = j) I(z_{rt}^{(k)} = i) \right) \]

\[ p_i \mid \sim \text{Dir} \left( \tilde{v}_1, \ldots, \tilde{v}_C \right), \; \tilde{v}_i = v_i + \frac{1}{T} \left( \sum_{k=1}^{K} \sum_{r \in U} \sum_{t=1}^{T} I(z_{rt}^{(k)} = i) \right) \]

A.2 Proofs

Proof of Theorem 1

For clarity, we prove the results assuming that \( n = \alpha N \), as the proof is similar when the relationship only holds in the limiting sense. For \( 0 \leq \alpha \leq 1 \), we have

\[ \ell_{U,N}(\theta) = -\frac{1}{N} \sum_{r=1}^{N} \sum_{j=1}^{C} a_{rj} \log \left( \sum_{i=1}^{C} \frac{M_{ij} p_i}{a_{rj}} \right) \]

\[ \ell_{L,n}(\tilde{M}) = -\frac{1}{N} \sum_{r=1}^{\alpha N} \sum_{j=1}^{C} a_{rj} \log \left( \sum_{i=1}^{C} \frac{M_{ij} b_i}{a_{rj}} \right) \]

and defining \( f_N = \ell_{U,N}(\theta) + \ell_{L,n}(\tilde{M}) \) our generalized posterior distribution is given by \( \nu_N = \Pi_N(d\theta) \propto \exp(-Nf_N(\theta))\Pi(d\theta) \). We now note that for any fixed \( M \), \( \lim_{N \to \infty} \ell_{L,n}(\tilde{M}) = \ell_{L}(\tilde{M}) \), as

\[ \ell_{L,n}(\tilde{M}) = -\frac{1}{N} \sum_{r=1}^{\alpha N} \sum_{j=1}^{C} a_{rj} \log \left( \sum_{i=1}^{C} \frac{M_{ij} b_i}{a_{rj}} \right) \]

\[ = \frac{N \alpha}{N} \sum_{r=1}^{\alpha N} \sum_{j=1}^{C} a_{rj} \log \left( \sum_{i=1}^{C} \frac{M_{ij} b_i}{a_{rj}} \right) \]

\[ \xrightarrow{N \to \infty} \alpha E_{r \in L} \left[ \sum_{j=1}^{C} a_{rj} \log \left( \sum_{i=1}^{C} \frac{M_{ij} b_i}{a_{rj}} \right) \right] \]

\[ = \alpha E_{L} \left[ D_{KL}(a||M\ b) \right] \]

\[ = \ell_{L}(\tilde{M}) \]
We will prove Lemma 1 by showing that

(i) $\ell_{L,n}$ is convex

(ii) $\nabla \ell_L(\tilde{M}^0) = 0$

(iii) $\nabla^2 \ell_L(\tilde{M}^0)$ exists and is positive definite.

We begin by proving (i) by showing that the Hessian $H_N$ of $\ell_{L,n}(\tilde{M}) > 0$. We have

$$
\frac{\partial \ell_{L,n}}{\partial M_{ij}} = -\frac{1}{N} \sum_{r=1}^{N} \left[ \frac{a_{ij,b_{ri}}}{\sum_{i=1}^{C} M_{ij} b_{ri}} \right]
$$

$$
\frac{\partial^2 \ell_{L,n}}{\partial M_{ij} \partial M_{i'j'}} = I(j = j') \frac{1}{N} \sum_{r=1}^{N} \frac{a_{ij,b_{ri}}b_{i'r'}}{\left( \sum_{i=1}^{C} M_{ij} b_{ri} \right)^2} + \frac{1}{N} \sum_{r=1}^{N} \frac{a_{iC,b_{ri}b_{i'r'}}}{\left( \sum_{i=1}^{C} M_{iC} b_{ri} \right)^2}
$$

Letting $v_{rj} = \frac{\sqrt{\pi_n}}{\sum_{i=1}^{C} M_{ij} b_{ri}} b_r$ and $V_j = (v_{ij}, \ldots, v_{(N\alpha)_j})$, and reorganizing the entries of $\tilde{M}$ in the order $M_{11}, M_{21}, \ldots, M_{C1}, M_{12}, \ldots, M_{C2}, \ldots, M_{C,C-1}$, we can write our Hessian $H_N$ as

$$
H_N = \frac{1}{N} \left( \begin{array}{cccc}
V_1 V_1' + V_C V_C' & V_C V_C' & \cdots & V_C V_C' \\
V_C V_C' & V_2 V_2' + V_C V_C' & \cdots & V_C V_C' \\
\vdots & \vdots & \ddots & \vdots \\
V_C V_C' & \cdots & \cdots & V_{C-1} V_{C-1}' + V_C V_C'
\end{array} \right)
$$

This implies that $H_N$ is singular if and only if there exists some $x \in \mathbb{R}^{C-1}$ and some $j$ such that $x' V_j = x' V_C = 0$. For each $j$, we rearrange the $v_{rj}$ such that

$$
V_j = \begin{pmatrix} B_{j,0} & B_j \end{pmatrix} \begin{pmatrix} 0 \\ A_j \end{pmatrix}
$$

where $A_j$ is a diagonal matrix with entries $\frac{\sqrt{\pi_n}}{\sum_{i=1}^{C} M_{ij} b_{ri}}$ on the diagonal for instances $r$ where $a_{rj} > 0$ and $B_{j,0}$ and $B_j$ correspond to the matrix of the $b_r's$ stacked as columns for instances $r \in L$ with $a_{rj} = 0$ and $a_{rj} > 0$, respectively. This allows us to write

$$
V_j = \begin{pmatrix} 0 & B_j A_j \end{pmatrix}
$$

which means that $V_j$ is full row rank if and only if $B_j$ is of full row-rank. By assumption 1, $B_j$ is full rank, and hence so is $V_j$, which is a sufficient condition for $H_N > 0$, which gives us that $\ell_{L,n}(\tilde{M})$ is convex.
To show condition (ii) holds, we see that

$$\frac{\partial \ell_L(\tilde{M})}{\partial M_{ij}} = -\alpha \frac{\partial}{\partial M_{ij}} \mathbb{E}_{r \in \mathcal{L}} \left[ \sum_j a_{rj} \log \left( \sum_i M_{ij}b_{ri} \right) \right]$$

To switch the order of differentiation and expectation, we will use the dominated convergence theorem and show that in a neighborhood of \( \tilde{M}^0 \)

$$\left| \frac{\partial}{\partial M_{ij}} a_{rj} \log \left( \sum_i M_{ij}b_{ri} \right) \right|$$

is bounded by some integrable random variable \( X \). We first note that

$$\left| \frac{\partial}{\partial M_{ij}} a_{rj} \log \left( \sum_i M_{ij}b_{ri} \right) \right| \leq \frac{b_{ri}}{\sum_{i=1}^C M_{ij}b_{ri}} + \frac{b_{ri}}{\sum_{i=1}^C M_{iC}b_{ri}}$$

and because \( \tilde{M}^0 \) is an interior point, we can choose a small enough neighborhood \( N_\epsilon(\tilde{M}^0) \) such that \( \forall \tilde{M} \in N_\epsilon(\tilde{M}^0), \min_{ij} M_{ij} > K \), where \( K \) is a constant that depends on \( \epsilon \) and \( \tilde{M}^0 \). Thus we have

$$\sum_{i=1}^C M_{ij}b_{ri} > K \sum_{i=1}^C b_{ri} = K \text{ implying that } \frac{a_{rj}b_{ri}}{\sum_{i=1}^C M_{ij}b_{ri}} < Ka_{rj}b_{ri}.$$  

And since \( a_{rj}b_{ri} \leq 1 \), the dominated convergence theorem applies. We now have

$$\frac{\partial \ell_L(\tilde{M})}{\partial M_{ij}} \bigg|_{\tilde{M}^0} = -\alpha \mathbb{E}_{r \in \mathcal{L}} \left[ \frac{a_{rj}b_{ri}}{\sum_{i=1}^C M_{ij}b_{ri}} - \frac{a_{rC}b_{ri}}{\sum_{i=1}^C M_{iC}b_{ri}} \right]$$

$$= -\alpha \mathbb{E}_{b_r, r \in \mathcal{L}, M^0 b_{ri}} \left[ E_{a_{rj}b_{ri}, r \in \mathcal{L}, M^0} \left[ \frac{a_{rj}b_{ri}}{\sum_{i=1}^C M_{ij}b_{ri}} - \frac{a_{rC}b_{ri}}{\sum_{i=1}^C M_{iC}b_{ri}} \right] \right]$$

$$= -\alpha \mathbb{E}_{b_r, r \in \mathcal{L}, M^0 b_{ri}} \left[ \sum_{i=1}^C M_{ij}b_{ri} \frac{a_{rj}b_{ri}}{\sum_{i=1}^C M_{ij}b_{ri}} - \sum_{i=1}^C M_{iC}b_{ri} \frac{a_{rC}b_{ri}}{\sum_{i=1}^C M_{iC}b_{ri}} \right]$$

$$= 0$$  \hspace{1cm} (A.1)

which proves (ii).

Moving to (iii), we appeal to the arguments made in the proof of (ii) to switch the orders of expectation and differentiation in a neighborhood of \( M^0 \). The fact that \( \sum_{i=1}^C \frac{1}{M_{ij}^0 b_{ri}} \geq \frac{1}{\max_{ij} M_{ij}^0} \) gives us

$$\frac{\partial^2 \ell_L(\tilde{M})}{\partial M_{ij} \partial M_{i'j'}} \bigg|_{M^0} = \mathbb{E}_{r \in \mathcal{L}} \left[ b_{ri}b_{r'j'} \left( \frac{I(j = j')}{\sum_{i=1}^C M_{ij}^0 b_{ri}} + \frac{1}{\sum_{i=1}^C M_{iC}^0 b_{ri}} \right) \right]$$
Because the Hessian $H$ dominates a block-diagonal matrix with blocks

$$H_j \geq \frac{1}{\max_{ij} M_{ij}} E_{r \in L} \left[ b_r b'_r \right] > 0$$

condition (iii) is proved. The three conditions (i) - (iii) are sufficient to establish Lemma 1 using Theorem 2.3 of Miller (2019).

Next we prove Lemma 2. We first note that

$$\ell_{\mathcal{U},N}(\tilde{\mathbf{M}}, \tilde{\mathbf{p}}) = \inf_{\tilde{q}} \ell_{\mathcal{U},N}(\tilde{\mathbf{M}}, \tilde{\mathbf{p}})$$

where

$$\tilde{\ell}_{\mathcal{U},N}(\tilde{q}) = \ell_{\mathcal{U},N}(\tilde{\mathbf{I}}, \tilde{q}) = -\frac{1}{N} \sum_{r=1}^{N} \sum_{j=1}^{C} a_{rj} \log(q_j) a_{rj}. \quad (A.2)$$

Clearly, $\tilde{\ell}_{\mathcal{U},N}(\tilde{q})$ is minimized at $\tilde{q}$ where

$$\hat{q}_j = \frac{1}{N} \sum_{r=1}^{N} a_{rj}. \quad \text{This proves Lemma 2 as}$$

$$\inf_{\theta \in \Theta} \ell_{\mathcal{U},N}(\tilde{\mathbf{M}}, \tilde{\mathbf{p}}) = \tilde{\ell}_{\mathcal{U},N}(\hat{q})$$

$$= -\sum_{j=1}^{C} \log(\hat{q}_j) \hat{q}_j + \frac{1}{N} \sum_{r=1}^{N} \sum_{j=1}^{C} a_{rj} \log(a_{rj})$$

$$\frac{N \to \infty}{-\sum_{j=1}^{C} \log(\sum_{i=1}^{C} M_{ij}^0 p_i^0)} - \sum_{j=1}^{C} \left[ \log(\sum_{i=1}^{C} M_{ij}^0 p_i^0) - E_{r \in \mathcal{U}} [a_{rj} \log(a_{rj})] \right]$$

$$= -\sum_{j=1}^{C} E_{r \in \mathcal{U}} \left[ a_{rj} \log\left( \sum_{i=1}^{C} M_{ij}^0 p_i^0 \right) \right]$$

$$= E_{\mathcal{U}} D_{KL}(a||M^0, p^0).$$

We now return to the loss function for the full data, $f_N$, to show

$$\liminf_{N} \inf_{\theta \notin B_{\epsilon}(\theta_0)} f_N(\theta) > f(\theta^0)$$

which would prove posterior consistency of the full generalized posterior. We first note that

$$\{||\theta - \theta^0||_2 > \epsilon\} \subseteq \{||\tilde{\mathbf{M}} - \tilde{\mathbf{M}}^0||_2 > h\} \cup \{||\tilde{\mathbf{p}} - \tilde{\mathbf{p}}^0||_2 > \epsilon/2, ||\tilde{\mathbf{M}} - \tilde{\mathbf{M}}^0||_2 < h\}$$

where $h < \epsilon/2$ is a fixed, but suitably small constant which we will specify later. We begin with the fact that

$$\lim \inf_{N} \inf_{\theta \notin B_{\epsilon}(\theta_0)} f_N(\theta) \geq \min\{\lim \inf_{N} \inf_{\theta \notin B_{h}(\tilde{\mathbf{M}} - \tilde{\mathbf{M}}^0)} f_N(\tilde{\mathbf{M}}, \tilde{\mathbf{p}}),$$

$$\lim \inf_{N} \inf_{\theta \notin B_{\epsilon/2}(\tilde{\mathbf{M}} - \tilde{\mathbf{M}}^0)} f_N(\tilde{\mathbf{M}}, \tilde{\mathbf{p}})\} \quad (A.3)$$

and will show that each of the two terms in the right hand side of (A.3) is greater than $f(\tilde{\mathbf{M}}^0, \tilde{\mathbf{p}}^0)$. Using Lemma 1(b) and Lemma 2 we immediately have

$$\lim \inf_{N} \inf_{\theta \notin B_{h}(\tilde{\mathbf{M}} - \tilde{\mathbf{M}}^0)} f_N(\tilde{\mathbf{M}}, \tilde{\mathbf{p}}) > f(\tilde{\mathbf{M}}^0, \tilde{\mathbf{p}}^0).$$
Focusing on the other term, we note that

\[ f_N(\tilde{M}, \tilde{p}) - f(\tilde{M}^0, \tilde{p}^0) = \ell_{L_n}(\tilde{M}) - \ell_{L}(\tilde{M}^0) + \ell_{U,N}(\tilde{M}, \tilde{p}) - \ell_{U,N}(\tilde{M}^0, \tilde{p}) + \ell_{U,N}(\tilde{M}^0, \tilde{p}) - \ell_{U}(\tilde{M}^0, \tilde{p}^0) \]

Letting \( A = \{|\tilde{p} - \tilde{p}^0|_2 < \epsilon/2, |\tilde{M} - \tilde{M}^0|_2 < h\} \) and using A.2 we have

\[ \liminf_N \inf_A f_N(\tilde{M}, \tilde{p}) - f(\tilde{M}^0, \tilde{p}^0) > -\limsup_N \sup_A |\ell_{L,n}(\tilde{M}^0) - \ell_{L,n}(\tilde{M}^0)| - \limsup_N |\ell_{U,n}(\tilde{M}^0) - \ell_{L}(\tilde{M}^0)| - \limsup_N \sup_A |\ell_{U,N}(\tilde{M}, \tilde{p}) - \ell_{U,N}(\tilde{M}^0, \tilde{p})| + \liminf_N \inf_{|\tilde{p} - \tilde{p}^0|_2 > \epsilon/2} \ell_{U,N}(\tilde{M}^0, \tilde{p}) - \ell_{U}(\tilde{M}^0, \tilde{p}^0) \]  

(A.4)

Note that the second term in A.2 is 0 as \( \ell_{L,n}(\tilde{M}^0) \to \ell_{L}(\tilde{M}^0) \). Focusing on the first term, we use the mean value theorem to have:

\[ \limsup_N \sup_A |\ell_{L,n}(\tilde{M}^0) - \ell_{L}(\tilde{M}^0)| \leq \limsup_N \sup_{\{|\tilde{M} - \tilde{M}^0|_2 < h\}} \max_{i,j} \frac{\partial \ell_{U,N}(\tilde{M})}{\partial M_{ij}} \left|\sum_{i,j} \frac{a_{ij}r_i}{M_{ij}} \right| \times \sup_{\{|\tilde{M} - \tilde{M}^0|_2 < h\}} |\tilde{M} - \tilde{M}^0|_1 \]

\[ \leq C h \times \limsup_N \sup_{\{|\tilde{M} - \tilde{M}^0|_2 < h\}} \max_{i,j} \frac{1}{N} \sum_{r=1}^{N_0} \left( \frac{a_{ij}b_r}{\sum_{i=1}^{N_0} M_{ij}b_r} + \frac{a_{ij}b_r}{\sum_{i=1}^{N_0} M_{ij}b_r} \right) \]

Since \( \tilde{M}^0 \) is an interior point, for small enough \( \epsilon \), we have \( \forall i, j, M_{ij} \geq K(\epsilon) \), and thus \( \sup_{\{|\tilde{M} - \tilde{M}^0|_2 < h\}} \sum_{i=1}^{N_0} \frac{1}{M_{ij}b_r} \leq \frac{1}{K(\epsilon)} \), which further implies

\[ \limsup_N \sup_A |\ell_{L,n}(\tilde{M}^0) - \ell_{L}(\tilde{M}^0)| \leq \limsup_N \frac{C h}{K(\epsilon)} \sum_{i,j} \frac{1}{N} \sum_{r=1}^{N_0} a_{ij}r_i \leq \frac{C^3 h}{K(\epsilon)} \cdot \]

Using the same logic as above, we also have

\[ \limsup_N \sup_A |\ell_{U,N}(\tilde{M}, \tilde{p}) - \ell_{U,N}(\tilde{M}^0, \tilde{p})| \leq \frac{C^3 h}{K(\epsilon)} \cdot \]

Combining this, we have

\[ \liminf_N \inf_A f_N(\tilde{M}, \tilde{p}) - f(\tilde{M}^0, \tilde{p}^0) > -\frac{2C^3 h}{K(\epsilon)} + \liminf_N \inf_{|\tilde{p} - \tilde{p}^0|_2 > \epsilon/2} \ell_{U,N}(\tilde{M}^0, \tilde{p}) - \ell_{U}(\tilde{M}^0, \tilde{p}^0) \]  

(A.5)

We define \( \ell^*_N(\tilde{p}) = \ell_{U,N}(\tilde{M}^0, \tilde{p}) \) which as \( N \to \infty \) goes to \( \ell^*(\tilde{p}) = \ell_{U}(\tilde{M}^0, \tilde{p}) \). First we will show that
\( \ell_{U,N}(\tilde{p}) \) is convex. We have

\[
\ell_{U,N}(\tilde{p}) = -\frac{1}{N} \sum_{r=1}^{N} \sum_{j=1}^{C} a_{rj} \log \left( \frac{\sum_{i=1}^{C} M_{ij}^0 p_i}{a_{rj}} \right)
\]

which implies

\[
\frac{\partial^2 \ell_{U,N}(\tilde{p})}{\partial p_i \partial p_i'} = \sum_{j=1}^{C} \hat{q}_j (M_{ij}^0 - M_{ij}^0 C_j) (M_{ij}^0 C_j - M_{ij}^0 C_j) \\
\left( \sum_{i=1}^{C} M_{ij}^0 p_i \right)^2
\]

Now letting

\[
D = \text{diag}(d_j) \quad \text{where} \quad d_j = \frac{\hat{q}_j}{\left( \sum_{i=1}^{C} M_{ij}^0 p_i \right)^2};
\]

\[
U = (u_1, \ldots, u_C) \text{ where } u_j = M_{i,(C-1),j}^0 - M_{Cj}^0 1_{C-1}
\]

we have \( \nabla^2 \ell_{U,N}(\tilde{p}) = \sum_{j=1}^{C} d_j u_j u_j' = UD' \). Now note that the rows of \( U \) are linear combinations of rows of \( M^0 \):

\[
U = \begin{pmatrix}
  e_1' - e_C' \\
  e_2' - e_C' \\
  \vdots \\
  e_{C-1}' - e_C'
\end{pmatrix} M^0
\]

And thus by assumption 2, that \( M^0 \) is full rank, \( U \) is also full rank and hence \( \ell_{U,N}(\tilde{p}) \) is convex.

Next, we now look at the properties of \( \nabla \ell_{U}(\tilde{p}^0) \) and \( \nabla^2 \ell_{U}(\tilde{p}^0) \). We have

\[
\ell_{U}(\tilde{p}) = -\sum_{j=1}^{C} \left[ E_{r \in U} \left[ \hat{q}_j \log(\sum_{i=1}^{C} M_{ij}^0 p_i) - a_{rj} \log(a_{rj}) \right] \right]
\]

\[
= -\sum_{j=1}^{C} \left[ \frac{\sum_{i=1}^{C} M_{ij}^0 p_i}{\left( \sum_{i=1}^{C} M_{ij}^0 p_i \right)^2} \left( \sum_{i=1}^{C} M_{ij}^0 p_i \right) - E_{r \in U} \left[ a_{rj} \log(a_{rj}) \right] \right] \quad (A.6)
\]

and thus

\[
\frac{\partial \ell_{U}(\tilde{p})}{\partial p_i} \bigg|_{\tilde{p} = \tilde{p}^0} = -\sum_{j=1}^{C} \frac{\sum_{i=1}^{C} M_{ij}^0 p_i}{\left( \sum_{i=1}^{C} M_{ij}^0 p_i \right)^2} (M_{ij}^0 - M_{Cj}^0)
\]

\[
= -\sum_{j=1}^{C} M_{ij}^0 + \sum_{j=1}^{C} M_{Cj}^0
\]

\[
= 0 \quad (A.7)
\]
And finally looking at $\nabla^2 \ell_\star U (\tilde{p}^0)$ we have

$$\nabla^2 \ell_\star U (\tilde{p}^0) \bigg|_{\tilde{p} = \tilde{p}^0} = UE_\star DU' > 0 \quad (A.8)$$

and thus by Theorem 2.3 of [Miller, 2019] we have

$$\liminf N \inf_{\{||p - \tilde{p}^0||_2 > \epsilon/2\}} \ell_\star U (\tilde{M}^0, \tilde{p}) - \ell_\star U (\tilde{M}^0, \tilde{p}^0) > \delta \quad (A.9)$$

for some $\delta > 0$. We now return to the constant $h$ and note that by choosing $h < \frac{\delta K(\epsilon)}{2C^3}$, we have

$$\liminf N \inf_A f_N(\tilde{M}, \tilde{p}) - f (\tilde{M}^0, \tilde{p}^0) > 0 \quad (A.10)$$

which completes the proof of Theorem 1. Corollary 2 is proved by simply extending the techniques used above to the case where each algorithm $k$ has its own misclassification matrix, $\tilde{M}^{(k)}$.

Turning our attention to Corollary 1, we denote the coarsened and rounded version of $f_N$ as $\tilde{f}_N$, using a factor $T_N$. As, $T_N \to \infty$, $\tilde{f}_N$ goes to the same pointwise limit $f$. We also have

$$\tilde{f}_N(\tilde{M}, \tilde{p}) - \tilde{f}_N(\tilde{M}, \tilde{p}) = -\frac{1}{N} \sum_{r=1}^{N} \sum_{j=1}^{C} \left( T_N \frac{a_{rj}}{T_N} - a_{rj} \right) \log \left( \sum_{i=1}^{C} M_{ij} p_i \right)$$

and because $\log \left( \sum_{i=1}^{C} M_{ij} p_i \right) < 0$, we have $\tilde{f}_N(\tilde{M}, \tilde{p}) \geq f_N(\tilde{M}, \tilde{p})$ which along with Theorem 1 shows

$$\liminf N \inf_{\theta \notin B_\epsilon(\theta_0)} \tilde{f}_N(\tilde{M}, \tilde{p}) > f (\tilde{M}^0, \tilde{p}^0) \quad (A.11)$$

References

Bella, A., Ferri, C., Hernández-Orallo, J., and Ramírez-Quintana, M. J. (2010). Quantification via probability estimators. In 2010 IEEE International Conference on Data Mining, pages 737–742. IEEE.

Bhattacharya, A., Pati, D., Yang, Y., et al. (2019). Bayesian fractional posteriors. The Annals of Statistics, 47(1):39–66.

Bissiri, P. G., Holmes, C. C., and Walker, S. G. (2016). A general framework for updating belief distributions. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 78(5):1103–1130.
Bragg, J., Weld, D. S., et al. (2013). Crowdsourcing multi-label classification for taxonomy creation. In *First AAAI conference on human computation and crowdsourcing*.

Byass, P., Chandramohan, D., Clark, S. J., D'ambruoso, L., Fottrell, E., Graham, W. J., Herbst, A. J., Hodgson, A., Hounton, S., Kahn, K., et al. (2012). Strengthening standardised interpretation of verbal autopsy data: the new interva-4 tool. *Global health action*, 5(1):19281.

Cole, S. R. and Stuart, E. A. (2010). Generalizing evidence from randomized clinical trials to target populations: The actg 320 trial. *American journal of epidemiology*, 172(1):107–115.

Comas-Cufí, M., Martín-Fernández, J. A., and Mateu-Figueras, G. (2016). Log-ratio methods in mixture models for compositional data sets. *SORT-Statistics and Operations Research Transactions*, 1(2):349–374.

Datta, A., Fiksel, J., Amouzou, A., and Zeger, S. (2018). Regularized bayesian transfer learning for population level etiological distributions. *Biostatistics (to appear)*.

Forman, G. (2005). Counting positives accurately despite inaccurate classification. In *European Conference on Machine Learning*, pages 564–575. Springer.

Forman, G. (2008). Quantifying counts and costs via classification. *Data Mining and Knowledge Discovery*, 17(2):164–206.

Giachanou, A. and Crestani, F. (2016). Like it or not: A survey of twitter sentiment analysis methods. *ACM Computing Surveys (CSUR)*, 49(2):28.

González, P., Castaño, A., Chawla, N. V., and Coz, J. J. D. (2017). A review on quantification learning. *ACM Computing Surveys (CSUR)*, 50(5):74.

Hijazi, R. H. and Jernigan, R. W. (2009). Modelling compositional data using dirichlet regression models. *Journal of Applied Probability & Statistics*, 4(1):77–91.

Hopkins, D. J. and King, G. (2010). A method of automated nonparametric content analysis for social science. *American Journal of Political Science*, 54(1):229–247.

Ibrahim, J. G., Chen, M.-H., Gwon, Y., and Chen, F. (2015). The power prior: theory and applications. *Statistics in medicine*, 34(28):3724–3749.

Kalter, H. D., Roubanatou, A.-M., Koffi, A., and Black, R. E. (2015). Direct estimates of national neonatal and child cause–specific mortality proportions in niger by expert algorithm and physician–coded analysis of verbal autopsy interviews. *Journal of global health*, 5(1).

Kessler, L. M. and Munkin, M. K. (2015). Bayesian estimation of panel data fractional response models with endogeneity: an application to standardized test rates. *Empirical Economics*, 49(1):81–114.

King, G., Lu, Y., et al. (2008). Verbal autopsy methods with multiple causes of death. *Statistical Science*, 23(1):78–91.
Li, Z., McCormick, T., and Clark, S. (2019). *openVA: Automated Method for Verbal Autopsy*. R package version 1.0.8.

Liang, K.-Y. and Zeger, S. L. (1986). Longitudinal data analysis using generalized linear models. *Biometrika*, 73(1):13–22.

McCormick, T. H., Li, Z. R., Calvert, C., Crampin, A. C., Kahn, K., and Clark, S. J. (2016). Probabilistic cause-of-death assignment using verbal autopsies. *Journal of the American Statistical Association*, 111(515):1036–1049.

McCullagh, P. and Nelder, J. (1989). *Generalized Linear Models, Second Edition*. Chapman and Hall/CRC Monographs on Statistics and Applied Probability Series. Chapman & Hall.

Miasnikof, P., Giannakeas, V., Gomes, M., Aleksandrowicz, L., Shestopaloff, A. Y., Alam, D., Tollman, S., Samarikhalaj, A., and Jha, P. (2015). Naive bayes classifiers for verbal autopsies: comparison to physician-based classification for 21,000 child and adult deaths. *BMC medicine*, 13(1):286.

Miller, J. W. (2019). Asymptotic normality, concentration, and coverage of generalized posteriors. *arXiv preprint arXiv:1907.09611*.

Miller, J. W. and Dunson, D. B. (2019). Robust bayesian inference via coarsening. *Journal of the American Statistical Association*, 114(527):1113–1125.

Moreno-Torres, J. G., Raeder, T., Alaiz-Rodríguez, R., Chawla, N. V., and Herrera, F. (2012). A unifying view on dataset shift in classification. *Pattern Recognition*, 45(1):521–530.

Mullahy, J. (2015). Multivariate fractional regression estimation of econometric share models. *Journal of Econometric Methods*, 4(1):71–100.

Murphy, K. P. et al. (2006). Naive bayes classifiers. *University of British Columbia*, 18:60.

Murray, C. J., Lopez, A. D., Black, R., Ajuha, R., Ali, S. M., Baqui, A., Dandona, L., Dantzer, E., Das, V., Dhingra, U., et al. (2011). Population health metrics research consortium gold standard verbal autopsy validation study: design, implementation, and development of analysis datasets. *Population health metrics*, 9(1):27.

Papke, L. E. and Wooldridge, J. M. (1996). Econometric methods for fractional response variables with an application to 401 (k) plan participation rates. *Journal of applied econometrics*, 11(6):619–632.

Pérez-Gállego, P., Castano, A., Quevedo, J. R., and del Coz, J. J. (2019). Dynamic ensemble selection for quantification tasks. *Information Fusion*, 45:1–15.

Serina, P., Riley, I., Stewart, A., James, S. L., Flaxman, A. D., Lozano, R., Hernandez, B., Mooney, M. D., Luning, R., Black, R., et al. (2015). Improving performance of the tariff method for assigning causes of death to verbal autopsies. *BMC medicine*, 13(1):291.
Specht, D. F. (1990). Probabilistic neural networks. *Neural networks*, 3(1):109–118.

Stan Development Team (2019). RStan: the R interface to Stan. R package version 2.19.2.

Szczurek, E., Biecek, P., Tiuryn, J., and Vingron, M. (2010). Introducing knowledge into differential expression analysis. *Journal of Computational Biology*, 17(8):953–967.

Tang, Z.-Z. and Chen, G. (2018). Zero-inflated generalized dirichlet multinomial regression model for microbiome compositional data analysis. *Biostatistics*.

Teicher, H. (1963). Identifiability of finite mixtures. *The annals of Mathematical statistics*, pages 1265–1269.

Valdez, A., Hancock, E. E., Adebayo, S., Kiernicki, D., Proskauer, D., Attewell, J. R., Bateman, L., DeMaria Jr, A., Lapp, C. W., Rowe, P. C., et al. (2018). Estimating prevalence, demographics and costs of me/cfs using large scale medical claims data and machine learning. *Frontiers in pediatrics*, 6:412.

Westreich, D., Edwards, J. K., Lesko, C. R., Stuart, E., and Cole, S. R. (2017). Transportability of trial results using inverse odds of sampling weights. *American journal of epidemiology*, 186(8):1010–1014.

Wong, T.-T. (1998). Generalized dirichlet distribution in bayesian analysis. *Applied Mathematics and Computation*, 97(2-3):165–181.

Yakowitz, S. J. and Spragins, J. D. (1968). On the identifiability of finite mixtures. *The Annals of Mathematical Statistics*, pages 209–214.

Yuan, Z., Chappell, R., and Bailey, H. (2007). The continual reassessment method for multiple toxicity grades: a bayesian quasi-likelihood approach. *Biometrics*, 63(1):173–179.