CORESETS FOR SCALABLE
BAYESIAN LOGISTIC REGRESSION

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ABSTRACT. The use of Bayesian models in large-scale data settings is attractive because of the rich hierarchical models, uncertainty quantification, and prior specification they provide. Standard Bayesian inference algorithms are computationally expensive, however, making their direct application to large datasets difficult or infeasible. Recent work on scaling Bayesian inference has focused on modifying the underlying algorithms to, for example, use only a random data subsample at each iteration. We leverage the insight that data is often redundant to instead obtain a weighted subset of the data (called a coreset) that is much smaller than the original dataset. We can then use this small coreset in any number of existing posterior inference algorithms without modification. In this paper, we develop an efficient coreset construction algorithm for Bayesian logistic regression models. We provide theoretical guarantees on the size and approximation quality of the coreset – both for fixed, known datasets, and in expectation for a wide class of data generative models. The proposed approach also permits efficient construction of the coreset in both streaming and parallel settings, with minimal additional effort. We demonstrate the efficacy of our approach on a number of synthetic and real-world datasets, and find that, in practice, the size of the coreset is independent of the original dataset size.

1. Introduction

Large-scale datasets, comprising tens or hundreds of millions of observations, are becoming the norm in scientific and commercial applications ranging from population genetics to advertising. At such scales even simple operations, such as examining each data point a small number of times, become burdensome; it is sometimes not possible to fit all data in the physical memory of a single machine. These constraints have, in the past, limited practitioners to relatively simple statistical modeling approaches. However, the rich hierarchical models, uncertainty quantification, and prior specification provided by Bayesian models have motivated substantial recent effort in making Bayesian inference procedures, which are often computationally expensive, scale to the large-data setting.

The standard approach to Bayesian inference for large-scale data is to modify a specific inference algorithm, such as MCMC or variational Bayes, to handle distributed or streaming processing of data. Examples include subsampling and streaming methods for variational Bayes [11, 12, 20], subsampling methods for MCMC [2, 7, 8, 22, 25, 33], and distributed “consensus” methods for MCMC [28, 30, 31]. Existing methods, however, suffer from both practical and theoretical limitations. Stochastic variational inference [20] and subsampling MCMC methods
require random access to the data, which is infeasible for very large datasets that do not fit into memory.

Furthermore, in practice, subsampling MCMC methods have been found to require examining a constant fraction of the data at each iteration, substantially limiting the computational gains obtained [3, 8, 9, 27, 32]. More scalable methods such as consensus MCMC [28, 30, 31] and streaming variational Bayes [11, 12] lead to substantial gains in computational efficiency, but lack rigorous justification and provide no guarantees on the quality of inference.

An important insight in the large-scale setting is that much of the data is often redundant, though there may also be a small set of data points that are distinctive. For example, in a large document corpus, one news article about a hockey game may serve as an excellent representative of hundreds or thousands of other similar pieces about hockey games. However, there may only be a few articles about luge, so it is also important to include at least one article about luge. Similarly, one individual’s genetic information may serve as a strong representative of other individuals from the same ancestral population admixture, though some individuals may be genetic outliers. We leverage data redundancy to develop a scalable Bayesian inference framework that modifies the dataset instead of the common practice of modifying the inference algorithm. Our method, which can be thought of as a preprocessing step, constructs a coreset — a small, weighted subset of the data that approximates the full dataset [1, 13] — that can be used in many standard inference procedures to provide posterior approximations with guaranteed quality. The scalability of posterior inference with a coreset thus simply depends on the coreset’s growth with the full dataset size. To the best of our knowledge, coresets have not previously been used in a Bayesian setting.

The concept of coresets originated in computational geometry (e.g. [1]), but then became popular in theoretical computer science as a way to efficiently solve clustering problems such as k-means and PCA (see [13, 15] and references therein). Coreset research in the machine learning community has focused on scalable clustering in the optimization setting [5, 6, 15, 24], with the exception of Feldman et al. [14], who developed a coreset algorithm for Gaussian mixture models. Coreset-like ideas have previously been explored for maximum likelihood-learning of logistic regression models, though these methods either lack rigorous justification or have only asymptotic guarantees (see [19] and references therein).

The job of the coreset in the Bayesian setting is to provide a approximation of the full data log-likelihood up to a multiplicative error uniformly over the parameter space. As this paper is the first foray into applying coresets in Bayesian inference, we begin with a theoretical analysis of the quality of the posterior distribution obtained from such an approximate log-likelihood. The remainder of the paper develops the efficient construction of small coresets for Bayesian logistic regression, a useful and widely-used model for the ubiquitous problem of binary classification. We develop a coreset construction algorithm, the output of which uniformly approximates the full data log-likelihood over parameter values in a ball with a user-specified radius. The approximation guarantee holds for a given dataset with high probability. We also obtain results showing that the boundedness of the parameter space is necessary for the construction of a nontrivial coreset, as well as results characterizing the algorithm’s expected performance under a wide class of data-generating distributions. Our proposed algorithm is applicable in both the
streaming and distributed computation settings, and the coreset can then be used by any inference algorithm which accesses the (gradient of the) log-likelihood as a black box. Although our coreset algorithm is specifically for logistic regression, we expect our approach and the methods we develop to be broadly applicable to other Bayesian generative models.

Experiments on a variety of synthetic and real-world datasets validate our approach and demonstrate robustness to the choice of algorithm hyperparameters. An empirical comparison to random subsampling shows that, in many cases, coreset-based posteriors are orders of magnitude better in terms of maximum mean discrepancy, including on a challenging 100-dimensional real-world dataset. All proofs are deferred to the Appendix.

2. Problem Setting

We begin with the general problem of Bayesian posterior inference. Let $D = \{(X_n, Y_n)\}_{n=1}^{N}$ be a dataset, where $X_n \in \mathcal{X}$ is a vector of covariates and $Y_n \in \mathcal{Y}$ is an observation. Let $\pi_0(\theta)$ be a prior density on a parameter $\theta \in \Theta$ and let $p(Y_n | X_n, \theta)$ be the likelihood of observation $n$ given the parameter $\theta$. The Bayesian posterior is given by the density

$$
\pi_N(\theta) := \frac{\exp(\mathcal{L}_N(\theta))\pi_0(\theta)}{\tilde{E}_N},
$$

(2.1)

where $\mathcal{L}_N(\theta) := \sum_{n=1}^{N} \ln p(Y_n | X_n, \theta)$ is the model log-likelihood and

$$
\tilde{E}_N := \int \exp(\mathcal{L}_N(\theta))\pi_0(\theta) \, d\theta
$$

(2.2)

is the marginal likelihood (a.k.a. the model evidence). Our aim is to construct a weighted dataset $\tilde{D} = \{ (\gamma_m, \tilde{X}_m, \tilde{Y}_m) \}_{m=1}^{M}$ with $M \ll N$ such that the weighted log-likelihood $\tilde{\mathcal{L}}_N(\theta) = \sum_{m=1}^{M} \gamma_m \ln p(\tilde{Y}_m | \tilde{X}_m, \theta)$ satisfies

$$
|\mathcal{L}_N(\theta) - \tilde{\mathcal{L}}_N(\theta)| \leq \varepsilon |\mathcal{L}_N(\theta)|, \quad \forall \theta \in \Theta.
$$

(2.3)

We call a weighted dataset $\tilde{D}$ that satisfies Eq. (2.3) an $\varepsilon$-coreset of $D$. If Eq. (2.3) holds, then the approximate posterior

$$
\tilde{\pi}_N(\theta) = \frac{\exp(\tilde{\mathcal{L}}_N(\theta))\pi_0(\theta)}{\tilde{E}_N}, \quad \text{with} \quad \tilde{E}_N = \int \exp(\tilde{\mathcal{L}}_N(\theta))\pi_0(\theta) \, d\theta
$$

(2.4)

has a marginal likelihood $\tilde{E}_N$ which approximates the true marginal likelihood $E_N$, as shown by Proposition 2.1. Thus, from a Bayesian perspective, the $\varepsilon$-coreset is a useful and meaningful notion of approximation.

**Proposition 2.1.** Let $\mathcal{L}(\theta)$ and $\tilde{\mathcal{L}}(\theta)$ be arbitrary non-positive log-likelihood functions that satisfy $|\mathcal{L}(\theta) - \tilde{\mathcal{L}}(\theta)| \leq \varepsilon |\mathcal{L}(\theta)|$ for all $\theta \in \Theta$. Then for any prior $\pi_0(\theta)$ such that the marginal likelihoods

$$
\mathcal{E} = \int \exp(\mathcal{L}(\theta))\pi_0(\theta) \, d\theta \quad \text{and} \quad \tilde{\mathcal{E}} = \int \exp(\tilde{\mathcal{L}}(\theta))\pi_0(\theta) \, d\theta
$$

(2.5)

are finite, the marginal likelihoods satisfy

$$
|\ln \mathcal{E} - \ln \tilde{\mathcal{E}}| \leq \varepsilon |\ln \mathcal{E}|.
$$

(2.6)
Algorithm 1: Construction of logistic regression coreset

Require: Data $\mathcal{D}$, $k$-clustering $Q$, radius $R > 0$, tolerance $\varepsilon \in (0, 1/4)$, failure rate $\delta \in (0, 1)$

1: for $n = 1, \ldots, N$ do $\triangleright$ calculate sensitivity upper bounds using the $k$-clustering

2: $m_n \leftarrow \left\lceil \frac{N}{1 + \sum_{i=1}^{k} |G_i|^{-R \|z_{G_i}^{(n)} - z_n\|_2}} \right\rceil$

3: end for

4: $\bar{m}_N \leftarrow \frac{1}{N} \sum_{n=1}^{N} m_n$

5: $M \leftarrow \left\lceil \frac{c}{\bar{m}_N^2} [D + 1 + \log(1/\delta)] \right\rceil$ $\triangleright$ coreset size

6: for $n = 1, \ldots, N$ do

7: $p_n \leftarrow \frac{m_n}{\bar{m}_N}$ $\triangleright$ importance weights of data

8: end for

9: $(K_1, \ldots, K_N) \sim \text{Multi}(M, (p_n)_n^{N})$ $\triangleright$ sample data for coreset

10: for $n = 1, \ldots, N$ do

11: $\gamma_n \leftarrow \frac{K_n}{p_n M}$ $\triangleright$ calculate coreset weights

12: end for

13: $\tilde{D} \leftarrow \{(\gamma_n, X_n, Y_n) \mid \gamma_n > 0\} \triangleright$ only keep data points with non-zero weights

14: return $\tilde{D}$

3. Coresets for Logistic Regression

3.1. Coreset Construction. In logistic regression, the covariates are real feature vectors $X_n \in \mathbb{R}^D$, the observations are labels $Y_n \in \{-1, 1\}$, $\Theta \subseteq \mathbb{R}^D$, and the likelihood is defined as

$$p(Y_n \mid X_n, \theta) = p_{\text{logistic}}(Y_n \mid X_n, \theta) := \frac{1}{1 + \exp(-Y_n X_n \cdot \theta)}.$$ (3.1)

The analysis in this work allows any prior $\pi_0(\theta)$; common choices are the Gaussian, Cauchy [16], and spike-and-slab [17, 26]. For notational brevity, we define $Z_n := Y_n X_n$, and let $\phi(s) := \ln(1 + \exp(-s))$. Choosing the optimal $\varepsilon$-coreset is not computationally feasible, so we take a less direct approach. We design our coreset construction algorithm and prove its correctness using a quantity $\sigma_n(\Theta)$ called the sensitivity [13], which quantifies the redundancy of a particular data point $n$ – the larger the sensitivity, the less redundant. In the setting of logistic regression, sensitivity is defined as

$$\sigma_n(\Theta) := \sup_{\theta \in \Theta} \frac{N \phi(Z_n \cdot \theta)}{\sum_{\ell=1}^{N} \phi(Z_{\ell} \cdot \theta)}.$$ (3.2)

Intuitively, $\sigma_n(\Theta)$ captures how much influence data point $n$ has on the log-likelihood $L_N(\theta)$ when varying the parameter $\theta \in \Theta$, and thus data points with high sensitivity should be included in the coreset. Evaluating $\sigma_n(\Theta)$ exactly is not tractable, however, so an upper bound $m_n \geq \sigma_n(\Theta)$ must be used in its place. Thus, the key challenge is to efficiently compute a tight upper bound on the sensitivity.

For the moment we will consider $\Theta = \mathbb{B}_R$ for any $R > 0$, where $\mathbb{B}_R := \{\theta \in \mathbb{R}^D \mid \|\theta\|_2 \leq R\}$; the case of $\Theta = \mathbb{R}^D$ will be discussed shortly. Choosing the parameter space to be a Euclidean ball is reasonable since data is usually preprocessed to have mean zero and variance 1 (or, for sparse data, to be between -1 and 1),
so each component of $\theta$ is typically in a range close to zero (e.g. between -4 and 4) [16].

The idea behind our sensitivity upper bound construction is that we would expect data points that are bunched together to be redundant while data points that are far from other data have a great effect on inferences. Clustering is an effective way to summarize data and detect outliers, so we will use a $k$-clustering of the data $D$ to construct the sensitivity bound. A $k$-clustering is given by $k$ cluster centers $Q = \{Q_1, \ldots, Q_k\}$. Let $G_i := \{Z_n \mid i = \arg\min_j \|Q_j - Z_n\|_2\}$ be the set of vectors closest to center $Q_i$ and let $G_i^{(-n)} := G_i \setminus \{Z_n\}$. Define $Z_{G,i}^{(-n)}$ to be a uniform random vector from $G_i^{(-n)}$ and let $\bar{Z}_{G,i}^{(-n)} := \mathbb{E}[Z_{G,i}^{(-n)}]$ be its mean. The following lemma uses a $k$-clustering to establish an efficiently computable upper bound on $\sigma_n(\mathbb{B}_R)$:

**Lemma 3.1.** For any $k$-clustering $Q$,

$$\sigma_n(\mathbb{B}_R) \leq m_n := \left[ \frac{N}{1 + \sum_{i=1}^k |G_i^{(-n)}|e^{-R\|\bar{Z}_{G,i}^{(-n)} - Z_n\|_2}} \right].$$  \hspace{1cm} \text{(3.3)}$$

Furthermore, $m_n$ can be calculated in $O(k)$ time.

The bound in Eq. (3.3) captures the intuition that if the data forms tight clusters, we expect each cluster to be well-represented by a small number of typical data points. Importantly, the bound can be computed efficiently in just $O(k)$ time. The (normalized) sensitivity bounds obtained from Lemma 3.1 are used to form an importance distribution ($p_n)_{n=1}^N$, from which to sample the coreset. If $Z_n$ is sampled, then it has weight $\gamma_n$ proportional to $1/p_n$. The size of the coreset depends on the mean sensitivity bound, the desired error $\varepsilon$, and a quantity closely related to the VC dimension of $\theta \mapsto \phi(\theta \cdot Z)$, which we show is $D + 1$. Combining these pieces we obtain Algorithm 1. The following theorem established that Algorithm 1 is guaranteed to construct an $\varepsilon$-coreset with high probability.

**Theorem 3.2.** Fix $\varepsilon \in (0, 1/4)$, $\delta \in (0, 1)$, and $R > 0$. Consider a dataset $D$ with $k$-clustering $Q$. Then with probability at least $1 - \delta$, the output of Algorithm 1 with inputs $(D, Q, R, \varepsilon, \delta)$ is an $\varepsilon$-coreset of $D$ for logistic regression with parameter space $\Theta = \mathbb{B}_R$. Furthermore, Algorithm 1 runs in $O(Nk)$ time.

**Remark 3.3.** The coreset algorithm is efficient with an $O(Nk)$ running time. However, the algorithm requires a $k$-clustering, which must also be constructed. A high-quality clustering can be obtained cheaply via $k$-means++ in $O(Nk)$ time [4], although a coreset algorithm could also be used.

Examining Algorithm 1, we see that the coreset size $M$ is proportional to $\bar{m}_N^2$, where $\bar{m}_N = \frac{1}{N} \sum m_n$. So for $M$ to be smaller than $N$, at a minimum, $\bar{m}_N$ should satisfy $\bar{m}_N = o(\sqrt{N})$, and preferably $\bar{m}_N = O(1)$. Indeed, for the coreset size to be small, it is critical that (a) $\Theta$ is chosen such that the sensitivities $\sigma_n(\Theta)$ are nontrivial (that is, $\ll N$), (b) each upper bound $m_n$ is close to $\sigma_n(\Theta)$, and (c) ideally, that $\bar{m}_N$ is bounded by a constant. In Section 3.2, we address (a) by providing sensitivity lower bounds, thereby showing that the constraint $\Theta = \mathbb{B}_R$ is necessary for nontrivial sensitivities even for “typical” (i.e. non-pathological) data. We then apply our lower bounds to address (b) and show that our bound in Lemma 3.1 is nearly tight. In Section 3.3, we address (c) by establishing the expected performance of the bound in Lemma 3.1 for a wide class of data-generating distributions.
3.2. Sensitivity Lower Bounds. We now develop lower bounds on the sensitivity to demonstrate that essentially we must limit ourselves to bounded $\Theta$,\textsuperscript{1} thus making our choice of $\Theta = \mathbb{B}_R$ a natural one, and to show that the sensitivity upper bound from Lemma 3.1 is nearly tight.

We begin by showing that in both the worst case and the average case, for all $n$, $\sigma_n(\mathbb{R}^D) = N$, the maximum possible sensitivity – even when the $Z_n$ are arbitrarily close. Intuitively, the reason for the worst-case behavior is that if there is a separating hyperplane between a data point $Z_n$ and the remaining data points, and $\theta$ is in the direction of that hyperplane, then when $\|\theta\|_2$ becomes very large, $Z_n$ becomes arbitrarily more important than any other data point.

**Theorem 3.4.** For any $D \geq 3$, $N \in \mathbb{N}$ and $0 < \epsilon' < 1$, there exists $\epsilon > 0$ and unit vectors $Z_1, \ldots, Z_N \in \mathbb{R}^D$ such that for all pairs $n, n'$, $Z_n \cdot Z_{n'} \geq 1 - \epsilon'$, and for any $R > 0$,

$$\sigma_n(\mathbb{B}_R) \geq \frac{N}{1 + (N - 1)e^{-Re\sqrt{\epsilon'}}/4} \quad \forall n. \tag{3.4}$$

Hence $\sigma_n(\mathbb{R}^D) = N$.

The proof of Theorem 3.4 is based on choosing $N$ distinct unit vectors $V_1, \ldots, V_N \in \mathbb{R}^{D-1}$ and setting $\epsilon = 1 - \max_{n \neq n'} V_n \cdot V_{n'} > 0$. But what is a “typical” value for $\epsilon$? In the case of the vectors being uniformly distributed on the unit sphere, we have the following scaling for $\epsilon$ as $N$ increases:

**Proposition 3.5.** If $V_1, \ldots, V_N$ are independent and uniformly distributed on the unit sphere $S^D := \{v \in \mathbb{R}^D \mid \|v\| = 1\}$ with $D \geq 2$, then with high probability

$$1 - \max_{n \neq n'} V_n \cdot V_{n'} \geq C_D N^{-4/(D-1)}, \tag{3.5}$$

where $C_D$ is a constant depending only on $D$.

Furthermore, $N$ can be exponential in $D$ even with $\epsilon$ remaining very close to 1:

**Proposition 3.6.** For $N = \lceil \exp((1 - \epsilon)D/2) / \sqrt{2} \rceil$, and $V_1, \ldots, V_N$ i.i.d. such that $V_{ni} = \pm \frac{1}{\sqrt{D}}$ with probability 1/2, then with probability at least 1/2,

$$1 - \max_{n \neq n'} V_n \cdot V_{n'} \geq \epsilon. \tag{3.6}$$

Propositions 3.5 and 3.6 demonstrate that the data vectors $Z_n$ found in Theorem 3.4 are, in two different senses, “typical” vectors and should not be thought of as worst-case data only occurring in some “negligible” or zero-measure set. These three results thus demonstrate that it is necessary to restrict attention to bounded $\Theta$. We can also use Theorem 3.4 to show that our sensitivity upper bound is nearly tight.

**Corollary 3.7.** For the data $Z_1, \ldots, Z_N$ from Theorem 3.4,

$$\frac{N}{1 + (N - 1)e^{-Re\sqrt{\epsilon'}}/4} \leq \sigma_n(\mathbb{B}_R) \leq \frac{N}{1 + (N - 1)e^{-Re\sqrt{2\epsilon'}}}. \tag{3.7}$$

\textsuperscript{1}Certain pathological choices of $\Theta$ could possibly be made that would be unbounded.
3.3. $k$-Clustering Sensitivity Bound Performance. While Lemma 3.1 and Corollary 3.7 provide an upper bound on the sensitivity given a fixed dataset, we would also like to understand how the expected mean sensitivity increases with $N$. We might expect it to be finite since the logistic regression likelihood model is parametric; the coreset would thus be acting as a sort of approximate finite sufficient statistic. Proposition 3.8 characterizes the expected performance of the upper bound from Lemma 3.1 under a wide class of generating distributions. This result demonstrates that, under reasonable conditions, the expected value of $\bar{m}_N$ is bounded for all $N$. As a concrete example, Corollary 3.9 specializes Proposition 3.8 to data with an underlying Gaussian generating distribution.

**Proposition 3.8.** Let $X_n \overset{\text{indep}}{\sim} N(\mu_{L_n}, \Sigma_{L_n})$, where $L_n \overset{\text{indep}}{\sim} \text{Multi}(\pi_1, \pi_2, \ldots)$ is the mixture component responsible for generating $X_n$. For $n = 1, \ldots, N$, let $Y_n, \bar{X}_n \in \{-1, 1\}$ be conditionally independent given $X_n$ and set $Z_n = Y_n X_n$. Select $0 < r < 1/2$, and define $\bar{\eta}_i = \max(\pi_i - N^{-r}, 0)$. The clustering of the data implied by $(L_n)_{n=1}^N$ results in the expected sensitivity bound

$$
\mathbb{E}[\bar{m}_N] \leq \frac{1}{N^{-1} + \sum_i \bar{\eta}_i e^{-R \sqrt{A_i N^{-\eta_i}} + B_i} + \sum_{i: \eta_i > 0} N e^{-2N^{1-2r}}} \quad (3.8)
$$

where

$$
A_i := \text{Tr}[\Sigma_i] + (1 - \bar{y}_i^2) \mu_i^T \mu_i, \quad B_i := \sum_j \bar{\pi}_j \left( \text{Tr}[\Sigma_j] + \bar{y}_j^2 \mu_i^T \mu_i - 2\bar{y}_i \bar{y}_j \mu_i^T \mu_j + \mu_i^T \mu_j \right),
$$

and $\bar{y}_i = \mathbb{E}[Y_1|L_1 = j]$.

**Corollary 3.9.** In the setting of Proposition 3.8, if $\pi_1 = 1$ and all data is assigned to a single cluster, then there is a constant $C$ such that for sufficiently large $N$,

$$
\mathbb{E}[\bar{m}_N] \leq C e^{R \sqrt{\text{Tr}[\Sigma_i] + (1 - \bar{y}_i^2) \mu_i^T \mu_i}}. \quad (3.10)
$$

### 3.4. Streaming and Parallel Settings

Algorithm 1 is a batch algorithm, but it can easily be used in parallel and streaming computation settings using standard methods from the coreset literature, which are based on the following two observations (cf. [14, Section 3.2]):

1. If $\bar{D}_i$ is an $\varepsilon$-coreset for $D_i$, $i = 1, 2$, then $\bar{D}_1 \cup \bar{D}_2$ is an $\varepsilon$-coreset for $D_1 \cup D_2$.
2. If $\bar{D}$ is an $\varepsilon$-coreset for $D$ and $\bar{D}'$ is an $\varepsilon'$-coreset for $\bar{D}$, then $\bar{D}'$ is an $\varepsilon''$-coreset for $\bar{D}$, where $\varepsilon'' := (1 + \varepsilon)(1 + \varepsilon') - 1$.

We can use these observations to merge coresets that were constructed either in parallel, or sequentially, in a binary tree. Coresets are computed for two data blocks, merged using observation 1, then compressed further using observation 2. The next two data blocks have coresets computed and merged/compressed in the same manner, then the coresets from blocks 1&2 and 3&4 can be merged/compressed analogously. We continue in this way and organize the merge/compress operations into a binary tree. Then, if there are $B$ data blocks total, only log $B$ blocks ever need be maintained simultaneously. In the streaming setting we would choose blocks of constant size, so $B = O(N)$, while in the parallel setting $B$ would be the number of machines available.
4. Experiments

We evaluated the performance of the logistic regression coreset algorithm on a number of synthetic and real-world datasets.

**Synthetic Binary Data.** We generated synthetic binary data according to the model \( X_{nd} \sim \text{Bern}(p_d), d = 1, \ldots, D \) and \( Y_n \sim \text{p}_{\text{logistic}}(\cdot | X_n, \theta) \). The idea is to simulate data in which there are a small number of rarely occurring but highly predictive features, which is a common real-world phenomenon. We thus took \( p = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10) \) for the \( D = 10 \) experiments and the first 5 components of \( p \) and \( \theta \) for the \( D = 5 \) experiments. The generative model is the same one used by Scott et al. \cite{30} and the first 5 components of \( p \) and \( \theta \) correspond to those used in the Scott et al. experiments (given in \cite[Table 1(b)]{30}).

**Synthetic Mixture Data.** We generated synthetic data with continuous covariates using a model similar to that of Han et al. \cite{19}: \( Y_n \sim \text{Bern}(1/2) \) and \( X_n \sim \mathcal{N}(\mu_c, I) \), where \( \mu_c = (0, 0, 0, 0, 1, 1, 1, 1) \) and \( \mu_1 = (1, 1, 1, 1, 1, 0, 0, 0, 0, 0) \).

**Chemical Reactivity Data.** The chemical reactivity dataset \cite{2} consists of \( N = 26,733 \) chemicals, each with \( D = 100 \) properties. The goal is to predict whether each chemical is reactive.

**Webspam Data.** The webspam corpus \cite{3} consists of \( N = 350,000 \) web pages, approximately 60% of which are spam. The covariates consist of the \( D = 127 \) features that each appear in at least 25 documents.

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\(^2\)Dataset ds1.100 obtained from http://komarix.org/ac/ds/.

\(^3\)http://www.cc.gatech.edu/projects/doi/WebbSpamCorpus.html
The running time was fast and comparable to that required for the clustering step, which was run using the implementation provided with scikit-learn ensuring that mean sensitivity is robust to the number of clusters $k$ it determines how the size of the coreset needs to scale with the data. Furthermore, an important empirical question is how the mean sensitivity $\bar{4.1}$. For example, the coreset algorithm took 2.5 seconds to run on our largest dataset, webspam, using a 2012 MacBook Pro with a 2.9 GHz Intel Core i7. We implemented the logistic regression coreset algorithm in Python and Cython. (a) binary data ($D = 5$) (b) binary data ($D = 10$) (c) mixture data ($D = 10$) (d) Reactivity data (e) Webspam data

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figs/corest}
\caption{Polynomial MMD and test log-likelihood of random sampling and the logistic regression coreset algorithm for synthetic and real data with varying subset sizes. For the synthetic data, $N = 10^6$ total data points were used and $10^4$ additional data points were generated for testing. For the real data, 2,500 (resp. 50,000) data points of the reactivity (resp. webspam) dataset were held out for testing.}
\end{figure}

We implemented the logistic regression coreset algorithm in Python and Cython. The running time was fast and comparable to that required for the $k$-means++ clustering step, which was run using the implementation provided with scikit-learn. For example, the coreset algorithm took 2.5 seconds to run on our largest dataset, webspam, using a 2012 MacBook Pro with a 2.9 GHz Intel Core i7.

4.1. Scaling Properties of the Coreset Construction Algorithm. An important empirical question is how the mean sensitivity $\bar{m}_p$ scales with $N$ because it determines how the size of the coreset needs to scale with the data. Furthermore, ensuring that mean sensitivity is robust to the number of clusters $k$ is critical since needing to adjust the algorithm hyperparameters for each dataset could lead to
an unacceptable increase in computational burden. We also seek to understand how the radius $R$ affects the mean sensitivity, the other coreset algorithm hyperparameter. Fig. 1 shows the results of our scaling experiments on synthetic binary data ($D = 10$) and the webspam data. The mean sensitivity is essentially constant across a range of dataset sizes, except for larger values of $R$. For both datasets the mean sensitivity is robust to the choice of $k$. But it scales exponentially in $R$, as we would expect from Lemma 3.1.

4.2. Posterior Approximation Quality. Since the ultimate goal is to use coresets for efficient Bayesian inference, the key empirical question is how well a posterior formed using a coreset approximates the true posterior distribution. We compared the coreset algorithm to random subsampling of data points, since that is the approach used in many existing scalable versions of variational inference and MCMC [7, 8, 20, 22]. Indeed, coreset-based importance sampling could be used as a drop-in replacement for the random subsampling used by these methods, though we leave the investigation of this idea for future work.

Experimental Setup. Posterior inference was done with an adaptive Metropolis-adjusted Langevin algorithm (MALA) [18, 29]. The coreset and random subsampling algorithms were each run 10 times for each choice of subsample size $M$. For the synthetic (resp. real-world) data, adaptive MALA was run once on the full dataset for 100,000 (resp. 200,000) iterations and for 20,000 (resp. 50,000) iterations for each approximate dataset produced by the coreset and random subsampling algorithms. All results are shown with $k = 50$ and $R = 2.5$. We obtained similar results for $30 \leq k \leq 100$ and $1.5 \leq R \leq 4.5$, indicating that the logistic regression coreset algorithm is robust to the choice of these hyperparameters. We used test log-likelihood and maximum mean discrepancy (MMD) with a polynomial kernel as comparison metrics.

Synthetic Data Results. Figures 2A-C show the results for synthetic data. In terms of test log-likelihood, coresets did as well as or outperformed random subsampling. In terms of MMD, the coreset posterior approximation typically outperformed random subsampling by 1-2 orders of magnitude and never did worse. These results suggest much can be gained by using coresets, with comparable performance to random subsampling in the worst case.

Real-world Data Results. Figures 2D and 2E show the results for real data. Coreset and random subsampling performance was approximately the same for webspam. While disappointing, it is important to note that using coresets does not lead to a worse posterior approximation. On the other hand, using coresets led to substantially better performance on the reactivity data, with a nearly optimal test log-likelihood obtained using only about 1,200 data points (about 5% of the full data size). Furthermore, on the reactivity data the coreset posterior MMD was many orders of magnitude smaller than the random subsampling posterior, which performed poorly even when a fairly large subsample was used (the slight deterioration in performance as the subsample size increases appears to be due to poor mixing).

For both the synthetic and real-world data, in most cases we are able to obtain a high-quality logistic regression posterior approximation using a coreset that is many orders of magnitude smaller than the full dataset – sometimes just a few dozen or hundred data points. Using such a small coreset represents a substantial reduction in the memory and computational requirements of the Bayesian inference
algorithm that uses the coreset for posterior inference. We expect that the use of coresets could lead similar gains for other Bayesian models. Designing coreset algorithms for other widely-used models is an exciting direction for future research.

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**Appendix A. Marginal Likelihood Approximation**

**Proof of Proposition 2.1.** By the assumption that $\mathcal{L}$ and $\tilde{\mathcal{L}}$ are non-positive, the multiplicative error assumption, and Jensen’s inequality,

$$\tilde{\mathcal{E}} = \int e^{\tilde{\mathcal{L}}(\theta)} \pi_0(\theta) \, d\theta \geq \int e^{(1+\varepsilon)\mathcal{L}(\theta)} \pi_0(\theta) \, d\theta \geq \left( \int e^{\mathcal{L}(\theta)} \pi_0(\theta) \, d\theta \right)^{1+\varepsilon} \cdots$$

and

$$\tilde{\mathcal{E}} = \int e^{\tilde{\mathcal{L}}(\theta)} \pi_0(\theta) \, d\theta \leq \int e^{(1-\varepsilon)\mathcal{L}(\theta)} \pi_0(\theta) \, d\theta \leq \left( \int e^{\mathcal{L}(\theta)} \pi_0(\theta) \, d\theta \right)^{1-\varepsilon} \cdots$$

\[ \square \]

**Appendix B. Main Results**

In order to construct coresets for logistic regression, we will use the framework developed by Feldman and Langberg [13]. For $n \in [N] := \{1, \ldots, N\}$, let $f_n : \mathcal{S} \to \mathbb{R}_+$ be a non-negative function from some set $\mathcal{S}$ and let $\bar{f} = \frac{1}{N} \sum_{n=1}^{N} f_n$ be the average of the functions. Define the sensitivity of $n \in [N]$ with respect to $\mathcal{S}$ by

$$\sigma_n(\mathcal{S}) := \sup_{s \in \mathcal{S}} \frac{f_n(s)}{\bar{f}(s)}, \quad (B.1)$$

and note that $\sigma_n(\mathcal{S}) \leq N$. Also, for the set $\mathcal{F} := \{f_n \mid n \in [N]\}$, define the dimension $\dim(\mathcal{F})$ of $\mathcal{F}$ to be the minimum integer $d$ such that

$$\forall F \subseteq \mathcal{F}, \ |\{F \cap R \mid R \in \text{ranges}(\mathcal{F})\}| \leq (|F| + 1)^d, \quad (B.2)$$

where $\text{ranges}(\mathcal{F}) := \{\text{range}(s, a) \mid s \in \mathcal{S}, a \geq 0\}$ and $\text{range}(s, a) := \{f \in \mathcal{F} \mid f(s) \leq a\}$.

**Theorem B.1 ([13, Theorems 4.1 and 4.4]).** Fix $\varepsilon \in (0, 1/4)$. For $n \in [N]$, let $m_n \in \mathbb{Z}_+$ be chosen such that

$$m_n \geq \sigma_n(\mathcal{S}) \quad (B.3)$$

and let $\bar{m}_N := \frac{1}{N} \sum_{n=1}^{N} m_n$. For $n \in [N]$, define the function $g_n = \bar{m}_N f_n / m_n$ and let the set $G_n$ consist of $m_n$ copies of $g_n$. There is a universal constant $c$ such that if $\mathcal{C}$ is a sample from $\mathcal{G} := \bigcup_{n=1}^{N} G_n$ of size

$$|\mathcal{C}| \geq \frac{c \bar{m}_N^2}{\varepsilon^2} \left( \dim(\mathcal{F}) + \ln(1/\delta) \right), \quad (B.4)$$

then with probability at least $1 - \delta$, for all $s \in \mathcal{S}$,

$$\left| N \bar{f}(s) - \frac{1}{|\mathcal{C}|} \sum_{g \in \mathcal{C}} g(s) \right| \leq \varepsilon N \bar{f}(s). \quad (B.5)$$
The set $C$ in the theorem is called a coreset. In our application to logistic regression, $S = \Theta$ and $f_n(\theta) = -\ln p(Y_n | X_n, \theta)$. The key is to determine $\dim(F)$ and to construct the values $m_n$ efficiently. Furthermore, it is necessary for $\bar{m}_N = O(\sqrt{N})$ at a minimum and preferable for $\bar{m}_N = O(1)$.

Letting $Z_n = Y_n X_n$ and $\phi(s) = \ln(1+\exp(-s))$, we can rewrite $f_n(\theta) = \phi(Z_n \cdot \theta)$. Hence, the goal is to find an upper bound

$$m_n \geq \sigma_n(\Theta) = \sup_{\theta \in \Theta} \frac{N \phi(Z_n \cdot \theta)}{\sum_{n'=1}^{N} \phi(Z_{n'} \cdot \theta)}.$$  

To obtain an upper bound on the sensitivity, we will take $\Theta = B_R$ for some $R > 0$.

**Lemma B.2.** For all $a, b \in \mathbb{R}$, $\phi(a)/\phi(b) \leq e^{a-b}$.

**Proof.** The lemma is trivial when $a = b$. Let $\Delta = b - a \neq 0$ and $\rho(a) = \phi(a)/\phi(a + \Delta)$. We have

$$\rho'(a) = \frac{(1 + e^a) \log(1 + e^{-a}) - (1 + e^{a+\Delta}) \log(1 + e^{-a-\Delta})}{(1 + e^a)(1 + e^{a+\Delta}) \log^2(1 + e^{-a-\Delta})}.$$  

(B.7)

Examining the previous display we see that $\text{sgn}(\rho'(a)) = \text{sgn}(\Delta)$. Hence if $\Delta > 0$,

$$\sup_a \frac{\phi(a)}{\phi(a + \Delta)} = \lim_{a \to \infty} \frac{\phi(a)}{\phi'(a)} = \lim_{a \to \infty} \frac{\phi'(a)}{\phi'(a + \Delta)} = \lim_{a \to \infty} \frac{e^{-a}}{1 + e^{-a}} \frac{1 + e^{-a-\Delta}}{e^{-a-\Delta}} = e^{\Delta} = e^{|b-a|},$$  

(B.11)

where the second equality follows from L’Hospital’s rule. Similarly, if $\Delta < 0$,

$$\sup_a \frac{\phi(a)}{\phi(a + \Delta)} = \lim_{a \to -\infty} \frac{e^{-a}}{1 + e^{-a}} \frac{1 + e^{-a-\Delta}}{e^{-a-\Delta}} = \lim_{a \to -\infty} \frac{e^{\Delta}}{e^{-a-\Delta}} = 1 \leq e^{|b-a|},$$  

(B.14)

where in this case we have used L’Hospital’s rule twice. □

**Lemma B.3.** The function $\phi(s)$ is convex.

**Proof.** A straightforward calculation shows that $\phi''(s) = \frac{e^s}{(1+e^s)^2} > 0$. □

**Lemma B.4.** For a random vector $Z \in \mathbb{R}^D$ with finite mean $\bar{Z} = \mathbb{E}[Z]$ and a fixed vector $V \in \mathbb{R}^D$,

$$\inf_{\theta \in \mathbb{B}_R} \mathbb{E} \left[ \frac{\phi(Z \cdot \theta)}{\phi(V \cdot \theta)} \right] \geq e^{-R\|\bar{Z} - V\|_2}.$$  

(B.15)
Proof. Using Lemmas B.2 and B.3 and Jensen’s inequality, we have
\[
\inf_{\theta \in \mathbb{R}} \mathbb{E}\left[ \frac{\phi(Z \cdot \theta)}{\phi(V \cdot \theta)} \right] \geq \inf_{\theta \in \mathbb{R}} \frac{\phi(\mathbb{E}[Z] \cdot \theta)}{\phi(V \cdot \theta)} \geq \inf_{\theta \in \mathbb{R}} e^{-|Z-V| \cdot \theta} = \inf_{\theta \in \mathbb{R}} e^{-R \|Z-V\|_2},
\]
(B.16)
(B.17)
(B.18)

Proof of Lemma 3.1. Straightforward manipulations followed by an application of Lemma B.4 yield
\[
\sigma_n(B_R)^{-1} = \inf_{\theta \in \mathbb{R}} \frac{1}{N} \sum_{n'=1}^{N} \frac{\phi(Z_n' \cdot \theta)}{\phi(Z_n \cdot \theta)} = \inf_{\theta \in \mathbb{R}} \frac{1}{N} \left[ 1 + \sum_{i=1}^{k} \sum_{Z \in G_i^{(-n)}} \frac{\phi(Z' \cdot \theta)}{\phi(Z_n \cdot \theta)} \right] \geq \frac{1}{N} \left[ 1 + \sum_{i=1}^{k} |G_i^{(-n)}| e^{-R \|Z_{G,i}^{(-n)}-Z_n\|_2} \right].
\]
(B.19)
(B.20)
(B.21)
(B.22)

To see that the bound can be calculated in \(O(k)\) time, first note that the cluster \(i_n\) to which \(Z_n\) belongs can be found in \(O(k)\) time while \(\bar{Z}_{G,i}^{(-n)}\) can be calculated in \(O(1)\) time. For \(i \neq i_n\), \(G_i^{(-n)} = G_i\), so \(\bar{Z}_{G,i}^{(-n)}\) is just the mean of cluster \(i\), and no extra computation is required. Finally, computing the sum takes \(O(k)\) time.
\(\square\)

In order to obtain an algorithm for generating coresets for logistic regression, we require a bound on the dimension of the range space constructed from the examples and logistic regression likelihood.

Proposition B.5. The set of functions \(\mathcal{F} = \{f_n(\theta) = \phi(Z_n \cdot \theta) \mid n \in [N]\}\) satisfies
\[
\dim(\mathcal{F}) \leq D + 1.
\]

Proof. For all \(F \subseteq \mathcal{F}\),
\[
|\{F \cap R \mid R \in \text{ranges}(\mathcal{F})\}| = |\{\text{range}(F, \theta, a) \mid \theta \in \Theta, a \geq 0\}|,
\]
(B.23)
where \(\text{range}(F, \theta, a) := \{f_n \in F \mid f_n(\theta) \leq a\}\). But, since \(\phi\) is invertible and monotonic,
\[
\{f_n \in F \mid f_n(\theta) \leq a\} = \{f_n \in F \mid \phi(Z_n \cdot \theta) \leq a\} = \{f_n \in F \mid Z_n \cdot \theta \leq \phi^{-1}(a)\},
\]
(B.24)
(B.25)
which is exactly a set of points shattered by the hyperplane classifier \(Z \mapsto \text{sgn}(Z \cdot \theta - b)\), with \(b := \phi^{-1}(a)\). Since the VC dimension of the hyperplane concept class
is $D + 1$, it follows that \cite{lemmas3.1 and 3.2}
\[
|\text{range}(F, \theta, a) | \theta \in \Theta, a \geq 0 | \leq \sum_{j=0}^{D+1} \left( |F| \right) \leq \sum_{j=0}^{D+1} \left( \frac{|F|}{j} \right) \tag{B.26}
\]
\[
\leq \sum_{j=0}^{D+1} \left( \frac{D+1}{j} \right) |F|^j = (|F| + 1)^{D+1}. \tag{B.27}
\]

**Proof of Theorem 3.2.** Combine Theorem B.1, Lemma 3.1, and Proposition B.5. The algorithm has overall complexity $O(Nk)$ since it requires $O(Nk)$ time to calculate the sensitivities by Lemma 3.1 and $O(N)$ time to sample the coreset. \hfill \Box

### Appendix C. Sensitivity Lower Bounds

**Lemma C.1.** Let $V_1, \ldots, V_K \in \mathbb{R}^{D-1}$ be unit vectors such that for some $\epsilon > 0$, for all $k \neq k'$, $V_k \cdot V_{k'} \leq 1 - \epsilon$. Then for $0 < \delta < \sqrt{1/2}$, there exist unit vectors $Z_1, \ldots, Z_K \in \mathbb{R}^D$ such that

- for $k \neq k'$, $Z_k \cdot Z_{k'} \geq 1 - 2\delta^2 > 0$
- for $k = 1, \ldots, K$ and $\alpha > 0$, there exists $\theta_k \in \mathbb{R}^D$ such that $\|\theta\|_2 \leq \sqrt{2\delta\alpha}$, $\theta_k \cdot Z_k = -\frac{\alpha\delta^2}{2}$ and for $k \neq k'$, $\theta_k \cdot Z_{k'} \geq \frac{\alpha\delta^2}{2}$.

**Proof.** Let $Z_k$ be defined such that $Z_{ki} = \delta V_{ki}$ for $i = 1, \ldots, D - 1$ and $Z_{kD} = \sqrt{1 - \delta^2}$. Thus, $\|Z_k\|_2 = 1$ and for $k \neq k'$,

\[
Z_k \cdot Z_{k'} = \delta^2 V_k \cdot V_{k'} + 1 - \delta^2 \geq 1 - 2\delta^2
\]
since $V_k \cdot V_{k'} \geq -1$. Let $\theta_k$ be such that $\theta_{ki} = -\alpha\delta V_{ki}$ for $i = 1, \ldots, D - 1$ and $\theta_{kd} = \frac{\alpha\delta^2(1 - \epsilon/2)}{\sqrt{1 - \delta^2}}$. Hence,

\[
\theta_k \cdot \theta_k = \alpha^2\delta^2 \left( V_k \cdot V_k + \frac{(1 - \epsilon/2)^2\delta^2}{1 - \delta^2} \right) \leq 2\alpha^2\delta^2
\]
\[
\theta_k \cdot Z_k = \alpha(-\delta^2 V_k \cdot V_k + \delta^2(1 - \epsilon/2)) = -\frac{\alpha\delta^2}{2},
\]
and for $k' \neq k$,

\[
\theta_k \cdot Z_{k'} = \alpha(-\delta^2 V_k \cdot V_{k'} + \delta^2(1 - \epsilon/2)) \geq \alpha\delta^2(1 + \epsilon + 1 - \epsilon/2) = \frac{\alpha\delta^2}{2}.
\]

\hfill \Box

**Proposition C.2.** Let $V_1, \ldots, V_K \in \mathbb{R}^{D-1}$ be unit vectors such that for some $\epsilon > 0$, for all $k \neq k'$, $V_k \cdot V_{k'} \leq 1 - \epsilon$. Then for any $0 < \epsilon' < 1$, there exist unit vectors $Z_1, \ldots, Z_K \in \mathbb{R}^D$ such that for $k, k'$, $Z_k \cdot Z_{k'} \geq 1 - \epsilon'$ but for any $R > 0$,

\[
\sigma_k(\mathbb{B}_R) \geq \frac{K}{1 + (K - 1)e^{-R\sqrt{\epsilon'/4}}}, \tag{C.1}
\]
and hence $\sigma_k(\mathbb{R}^D) = K$. 

Proof. Let $Z_1, \ldots, Z_K \in \mathbb{R}^D$ be as in Lemma C.1 with $\delta$ such that $\delta^2 = \epsilon'/2$. Since for $s \geq 0$, $\phi(s)/\phi(-s) \leq e^{-s}$, conclude that, choosing $\alpha$ such that $\sqrt{2} \alpha \delta = R$, we have

\[
\sigma_n(\mathbb{R}_R) = \sup_{\theta \in \mathbb{R}_R} \frac{K \phi(Z_k \cdot \theta)}{\sum_{k=1}^K \phi(Z_k \cdot \theta)} \\
\geq \frac{K \phi(-\alpha \delta^2/2)}{\phi(-\alpha \delta^2/2) + (K-1)\phi(\alpha \delta^2/2)} \\
\geq \frac{K}{1 + (K-1)e^{-\alpha \delta^2/2}} \\
= \frac{K}{1 + (K-1)e^{-Re\sqrt{\epsilon'}/2}}.
\]

Proof of Theorem 3.4. Choose $V_1, \ldots, V_N \in \mathbb{R}^{D-1}$ to be any $N$ distinct unit vectors. Apply Proposition C.2 with $K = N$ and $\epsilon = 1 - \max_{n \neq n'} V_n \cdot V_{n'} > 0$. □

Proof of Proposition 3.5. First note that if $V$ is uniformly distributed on $S^D$, then the distribution of $V \cdot V'$ does not depend on the distribution of $V'$ since $V \cdot V'$ and $V \cdot V''$ are equal in distribution for all $V', V'' \in S^D$. Thus it suffices to take $V_1' = 1$ and $V_i' = 0$ for all $i = 2, \ldots, D$. Hence the distribution of $V \cdot V'$ is equal to the distribution of $V_1$. The CDF of $V_1$ is easily seen to be proportional to the surface area (SA) of $C_s := \{v \in S^D | v_1 \leq s\}$. That is, $\mathbb{P}[V_1 \leq s] = \text{SA}(C_s)/\text{SA}(C_1)$. Let $U \sim \text{Beta}(\frac{D-1}{2}, \frac{1}{2})$, and let $B(a, b)$ be the beta function. It follows from [23, Eq. 1], that by setting $s = 1 - \epsilon$ with $\epsilon \in [0, 1/2]$,

\[
\mathbb{P}[V_1 \geq 1 - \epsilon] = \frac{1}{2} \mathbb{P}[-\sqrt{1-U} \leq \epsilon - 1] = \frac{1}{2} \mathbb{P}[U \leq 2\epsilon - \epsilon^2] \leq \frac{1}{2B(\frac{D-1}{2}, \frac{1}{2})} \int_0^{2\epsilon-\epsilon^2} t^{(D-3)/2}(1-t)^{-1/2} dt \leq \frac{1}{2B(\frac{D-1}{2}, \frac{1}{2})} (1-\epsilon)^{-1} \int_0^{2\epsilon-\epsilon^2} t^{(D-3)/2} dt \leq \frac{1}{2B(\frac{D-1}{2}, \frac{1}{2})} \frac{(2-\epsilon)^{(D-1)/2}}{1-\epsilon} e^{(D-1)/2} \leq \frac{1}{(D-1)B(\frac{D-1}{2}, \frac{1}{2})} e^{(D-1)/2}.
\]

Applying a union bound over the $\binom{D}{2}$ distinct vector pairs completes the proof. □

Lemma C.3 (Hoeffding’s inequality [10, Theorem 2.8]). Let $A_k$ be zero-mean, independent random variables with $A_k \in [-a, a]$. Then for any $t > 0$,

\[
\mathbb{P} \left( \sum_{k=1}^K A_k \geq t \right) \leq e^{-\frac{t^2}{2a^2K}}.
\]
Proof of Proposition 3.6. We say that unit vectors $V$ and $V'$ are $(1 - \epsilon)$-orthogonal if $|V \cdot V'| \leq 1 - \epsilon$. Clearly $\|V_n\|_2 = 1$. For $n \neq n'$, by Hoeffding’s inequality $\mathbb{P}(|V_n \cdot V_{n'}| \geq 1 - \epsilon) \leq 2e^{-(1-\epsilon)^2D/2}$. Applying a union bound to all $\binom{K}{2}$ pairs of vectors, the probability that any pair is not $(1 - \epsilon)$-orthogonal is at most
\[
2\binom{K}{2}e^{-(1-\epsilon)^2D/2} \leq \frac{1}{2}. \tag{C.9}
\]
Thus, with probability at least $1/2$, $V_1, \ldots, V_N$ are pairwise $(1 - \epsilon)$-orthogonal. \hfill \Box

Proof of Corollary 3.7. The data from Theorem 3.4 satisfies $Z_n \cdot Z_{n'} \geq 1 - \epsilon'$, so for $n \neq n'$,
\[
\|Z_n - Z_{n'}\|_2^2 = 2 - 2Z_n \cdot Z_{n'} \leq 2\epsilon'.
\]
Applying Lemma 3.1 with the clustering $Q = \{Z_1, \ldots, Z_N\}$ and combining it with the lower bound in Theorem 3.4 yields the result. \hfill \Box

Appendix D. A Priori Expected Sensitivity Upper Bounds

Proof of Proposition 3.8. First, fix the number of datapoints $N \in \mathbb{N}$. Since $X_n$ are generated from a mixture, let $L_n$ denote the integer mixture component from which $X_n$ was generated, let $C_i$ be the set of integers $1 \leq j \leq N$ with $j \neq n$ and $L_j = i$, and let $C = (C_i)_{i=1}^\infty$. Note that with this definition, $|G_i^{(-n)}| = |C_i|$. Using Jensen’s inequality and the upper bound from Lemma 3.1 with the clustering induced by the label sequence,
\[
\mathbb{E} [\sigma_n (B_R)] \leq \mathbb{E} [m_n] = NE \left[ \frac{1}{1 + \sum_i |C_i|e^{-R\|Z_{G,i}^{(-n)} - Z_n\|_2}} \right] \tag{D.1}
\]
\[
= NE \left[ \mathbb{E} \left[ \frac{1}{1 + \sum_i |C_i|e^{-R\|Z_{G,i}^{(-n)} - Z_n\|_2}} \bigg| C \right] \right] \tag{D.2}
\]
\[
\leq NE \left[ \frac{1}{1 + \sum_i |C_i|e^{-RE\|Z_{G,i}^{(-n)} - Z_n\|_2}} \right]. \tag{D.3}
\]
Using Jensen’s inequality again and conditioning on the labels $Y = (Y_n)_{n=1}^N$ and indicator $L_n$,
\[
\mathbb{E} \left[ \|Z_{G,i}^{(-n)} - Z_n\|_2 \big| C \right] \leq \sqrt{\mathbb{E} \left[ \|Z_{G,i}^{(-n)} - Z_n\|_2^2 \big| C \right]} \quad \tag{D.4}
\]
\[
= \sqrt{\mathbb{E} \left[ \mathbb{E} \left[ \|Z_{G,i}^{(-n)} - Z_n\|_2^2 \big| C, L_n, Y \right] \bigg| C \right]}. \quad \tag{D.5}
\]
For fixed labels $Y$ and clustering $C, L_n$, the linear combination in the expectation is multivariate normal with
\[
Z_{G,i}^{(-n)} - Z_n \sim N \left( \frac{1}{|C_i|} \left( \sum_{j \in C_i} Y_j \right), \frac{1}{|C_i|} \Sigma_i + \Sigma' \right). \tag{D.6}
\]
where $\mu'_i, \Sigma'_i$ are the mean and covariance of the mixture component that generated $X_n$. Further, for any multivariate normal random vector $W \in \mathbb{R}^n$,

$$
E[W^T W] = \sum_{m=1}^{d} E[W_m^2] = \sum_{m=1}^{d} \text{Var}[W_m] + E[W_m]^2, \quad (D.7)
$$

so

$$
E\left[\|Z_{G,i}^{(-n)} - Z_n\|_2^2 \mid L_n, C, Y\right] = \text{Tr}\left[\frac{1}{|C_i|} \Sigma_i + \Sigma'_n\right] + \left(\sum_{j \in C_i} \frac{Y_j}{|C_i|}\right)^2 \mu_i^T \mu_i - 2Y_n \left(\sum_{j \in C_i} \frac{Y_j}{|C_i|}\right) \mu_i^T \mu'_n + \mu'_n^T \mu'_n. \quad (D.8)
$$

Exploiting the i.i.d.-ness of $Y_j$ for $j \in C_i$ given $C$, defining $\bar{y}_j = E[Y_j \mid L_i = j]$, and noting that $X_n$ is sampled from the mixture model,

$$
E\left[\|Z_{G,i}^{(-n)} - Z_n\|_2^2 \mid L_n, C, Y\right] \mid C = \sum_j \pi_j \left(\text{Tr}\left[\frac{1}{|C_i|} \Sigma_i + \Sigma_j\right] + \left(\frac{|C_i|}{|C_i|}\right) \bar{y}_j^2 + \frac{1 - \bar{y}_j^2}{|C_i|} \mu_i^T \mu_i - 2\bar{y}_j \bar{y}_i \mu_i^T \mu_j + \mu_i^T \mu_j\right) \quad (D.9)
$$

$$
= \sum_j \pi_j \left(\text{Tr}[\Sigma_i] + \left(1 - \bar{y}_j^2\right) \mu_i^T \mu_i + \text{Tr}[\Sigma_j] + \bar{y}_j^2 \mu_i^T \mu_j - 2\bar{y}_j \bar{y}_i \mu_i^T \mu_j + \mu_i^T \mu_j\right) \quad (D.10)
$$

$$
= A_i |C_i|^{-1} + B_{in}, \quad (D.11)
$$

where $A_i$ and $B_i$ are positive constants

$$
A_i = \text{Tr}[\Sigma_i] + \left(1 - \bar{y}_j^2\right) \mu_i^T \mu_i \quad (D.12)
$$

$$
B_i = \sum_j \pi_j \left(\text{Tr}[\Sigma_j] + \bar{y}_j^2 \mu_i^T \mu_j - 2\bar{y}_j \bar{y}_i \mu_i^T \mu_j + \mu_i^T \mu_j\right). \quad (D.13)
$$

Therefore, with $0^{-1}$ defined to be $+\infty$,

$$
E[m_n] \leq N \mathbb{E}\left[\frac{1}{1 + \sum_i |C_i| e^{e^{-R\sqrt{A_i}|C_i|^{-1}+B_i}}}\right]. \quad (D.14)
$$

As $N \to \infty$, we expect the values of $|C_i|/N$ to concentrate around $\pi_i$. To get a finite sample bound using this intuition, we split the expectation into two conditional expectations: one where all $|C_i|/N$ are not too far from $\pi_i$, and one where they may be. Define $g : \mathbb{R}^\mathbb{R} \to \mathbb{R}_+$ as

$$
g(x) = \frac{1}{1 + \sum_i \sum_i e^{-R\sqrt{A_i|x_i|^{-1}+B_i}}}, \quad (D.15)
$$

$$
\pi = (\pi_1, \pi_2, \ldots), \quad \epsilon = (\epsilon_1, \epsilon_2, \ldots) \text{ with } \epsilon_i > 0, \text{ and } \eta = \max(\pi - \epsilon, 0). \text{ Then}
$$

$$
E[m_n] \leq N \mathbb{P}\left(\frac{|C_i|}{N} \geq \eta i\right) g(N\eta) + N \mathbb{P}\left(\exists i : \frac{|C_i|}{N} < \eta_i\right) \quad (D.16)
$$

$$
= Ng(N\eta) + N \mathbb{P}\left(\exists i : \frac{|C_i|}{N} < \eta_i\right) (1 - g(N\eta)). \quad (D.17)
$$
Using the union bound, noting that $1 - g(N\eta) \leq 1$, and then using Hoeffding’s inequality yields

\[
E[m_n] \leq N g(N\eta) + N \sum_i \Pr \left( \left| \frac{|C_i|}{N} - \pi_i \right| < \epsilon_i \right) \leq N g(N\eta) + N \sum_{i: \pi_i > \epsilon_i} e^{-2N\epsilon_i^2} \leq \frac{1}{N^{-1} + \sum_i \eta_i e^{-R\sqrt{A_i(N^{-1}\eta_i^{-1} + B_i)}} + \sum_{i: \pi_i > \epsilon_i} Ne^{-2N\epsilon_i^2}. \tag{D.20}
\]

We are free to pick $\epsilon$ as a function of $\pi$ and $N$. Let $\epsilon = N^{-r}$ for any $0 < r < 1/2$. Note that this means $\eta_i = \max(\pi_i - N^{-r}, 0)$. Then

\[
E[m_n] = \frac{1}{N^{-1} + \sum_i \eta_i e^{-R\sqrt{A_i(N^{-1}\eta_i^{-1} + B_i)}} + \sum_{i: \pi_i > \epsilon_i} Ne^{-2N\epsilon_i^2}} \tag{D.21}
\]

It is easy to see that the first term converges to $\left( \sum_i \pi_i e^{-R\sqrt{B_i}} \right)^{-1}$ by a simple asymptotic analysis. To show the second term converges to 0, note that for all $N$,

\[
\sum_i \pi_i = \sum_{i: \pi_i > N^{-r}} \pi_i + \sum_{i: \pi_i \leq N^{-r}} \pi_i \geq \sum_{i: \pi_i > N^{-r}} \pi_i \geq \sum_{i: \pi_i > N^{-r}} N^{-r} = \left| \{ i : \pi_i > N^{-r} \} \right| N^{-r}. \tag{D.22}
\]

Since $\sum_i \pi_i = 1 < \infty$, $\left| \{ i : \pi_i > N^{-r} \} \right| = O(N^r)$. Therefore there exists constants $C, M < \infty$ such that

\[
\left| \{ i : \pi_i > N^{-r} \} \right| \leq M + CN^r, \tag{D.23}
\]

and thus

\[
\sum_{i: \pi_i > N^{-r}} Ne^{-2N^{1-2r}} \leq N(M + CN^r)e^{-2N^{1-2r}} \to 0, \quad N \to \infty. \tag{D.24}
\]

Finally, since $\tilde{m}_N = \frac{1}{N} \sum_{n=1}^{N} m_n$, we have $E[\tilde{m}_N] = E[m_n]$, and the result follows.

**Proof of Corollary 3.9.** This is a direct result of Proposition 3.8 with $\pi_1 = 1, \pi_i = 0$ for $i \geq 2$. \qed

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