NO FREE LUNCH FOR APPROXIMATE MCMC

JAMES JOHNDROW, NATESH S. PILLAI, AND AARON SMITH

ABSTRACT. It is widely known that the performance of Markov chain Monte Carlo (MCMC) can degrade quickly when targeting computationally expensive posterior distributions, such as when the sample size is large. This has motivated the search for MCMC variants that scale well to large datasets. One general approach has been to look at only a subsample of the data at every step. In this note, we point out that well-known MCMC convergence results often imply that these “subsampling” MCMC algorithms cannot greatly improve performance. We apply these generic results to realistic statistical problems and proposed algorithms, and also discuss some design principles suggested by the results.

1. Introduction

Although they are ubiquitous in small-scale Bayesian inference, MCMC algorithms often perform poorly in “big data” – i.e. large sample size – problems. The simplest reason for this poor scaling is that most popular MCMC algorithms require a computation involving every data point at every time step. Ignoring the variation in speed of different types of computer memory, this suggests the heuristic that the per-step computational cost of MCMC scales linearly in the size $n$ of the data set.

There has been a great deal of recent work on methods to avoid this linear scaling by looking only at a few carefully-chosen control variates and a (possibly random) subsample of the data at every step. Much of this work was inspired by the still-recent paper [KCW14]. This note is an attempt to clarify what improvements are possible using methods similar to those currently being proposed. Our basic conclusion is similar to that of the recent paper [NDH+17], which studies natural upper bounds on the convergence rate in the important case of the stochastic gradient Langevin algorithm.

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johndrow@wharton.upenn.edu, Department of Statistics University of Pennsylvania, 3730 Walnut St, Philadelphia PA 19104, USA.

pillai@fas.harvard.edu, Department of Statistics Harvard University, 1 Oxford Street, Cambridge MA 02138, USA.

smith.aaron.matthew@gmail.com, Department of Mathematics and Statistics University of Ottawa, 585 King Edward Drive, Ottawa ON K1N 7N5, Canada.
Our main results, given in Theorems 3 and 4, apply to very general models and Markov chains, and give lower bounds on accuracy of Monte Carlo estimators (rather than merely lower bounds on natural upper bounds). One cost of this added generality and strength is that the results are somewhat technical to state precisely. For example, we need a careful notion of what it means to “use” a data point in the presence of pre-computed control variates. We therefore start by giving an informal summary of these results, followed by a somewhat more precise statement of a specific theorem applying to generalized linear models. Under various conditions which appear to apply to many statistical models and most of the subsampling algorithms that exist in the literature, our conclusion is that at least one of the following three things must happen:

1. The Markov chain mixes slowly enough that there is a very small overall computational cost advantage (though there may be a large per-step advantage); or
2. The stationary measure of the Markov chain is “far” from the posterior distribution conditioned on all data; or
3. The algorithm takes advantage of control variates that are very nearly sufficient statistics; i.e. one can obtain a very accurate approximation to the posterior by conditioning only on the control variates, without seeing the rest of the data.

The first two options amount to failure of a subsampling MCMC algorithm to meet its main goal of speeding up the computation of accurate posterior integrals. The third option requires very good low-dimensional control variates, which presents two more subtle problems. The first problem is practical: good control variates are often computationally expensive to construct, and this must be factored into the total computational cost of an algorithm. The second problem is related to motivation: once good control variates have been found, there is very little benefit to looking at the rest of the data, so one might as well run an algorithm using only the control variates and avoid the subsampling entirely. Thus, in all three cases, we find that there is a strong reason to avoid subsampling MCMC. Our results are quite general and explicitly apply to subsampling algorithms that use data augmentation or for which the invariant measure is not exactly the posterior distribution conditioned on the full dataset.

\footnote{In practice, it is not always easy to do posterior computations based on just control variates. The class of models for which this is difficult gives an important “way out” of our trilemma - see Section 1.3.}
Because the notion of computational cost is central to the paper, it is worth specifying at the outset exactly how we conceive of computational cost, which largely follows works such as [NDH+17, BPSW17]. The goal of MCMC is to obtain accurate approximations of expectations under the target measure. Consider a generic Markov chain $W_1, \ldots, W_N$ evolving according to a reversible Markov kernel $K_z$ depending on a dataset $z$ with $n$ data points with unique invariant measure $\pi_z$ and $L_2(\pi_z)$ spectral gap $\lambda_z$. Then for $\varphi \in L_2(\pi_z)$,

$$\sqrt{N} \left( \pi_z \varphi - N^{-1} \sum_{j=1}^{N} \varphi(W_j) \right) \rightsquigarrow N(0, \sigma^2_{\varphi,z}).$$

(1.1)

Thus the length of the path needed to achieve any desired approximation accuracy is proportional to the asymptotic variance $\sigma^2_{\varphi,z}$. A uniform upper bound on $\sigma^2_{\varphi,z}$ can be given in terms of $\lambda_z$

$$\sup_{\varphi \in L_2(\pi_z)} \frac{\sigma^2_{\varphi,z}}{\text{Var}_{\pi_z}(\varphi)} = \frac{2}{\lambda_z} - 1 \leq \frac{2}{\lambda_z}$$

(1.2)

The inverse of the spectral gap is referred to as the relaxation time. Thus if two MCMC algorithms have the same per-step computational cost, it is reasonable to compare their overall computational cost by comparing their relaxation times.

However, when considering subsampling algorithms, we are often comparing two MCMC algorithms with different per-step computational cost. To account for this, we introduce another quantity $\tau_z$, which is the number of steps necessary to “use” all $n$ data points at least once with high probability (we make “using data points” precise in Section 2.4). Like $\lambda_z$, this quantity depends on the data $z$, and this is the randomness at play in the “with high probability” statement in the definition of $\tau_z$. The overall computational cost of the algorithm is then (again with high probability)

$$\text{cost}(K_z) = \frac{n}{\lambda_z \tau_z},$$

(1.3)

since on average one uses at least $n/\tau_z$ data points to extend the Markov chain by one step.

For non-reversible $K_z$, this calculation can be done in terms of the pseudospectral gap $\lambda_z^{(ps)}$, but the upper bound in (1.2) with $\lambda_z$ replaced by $\lambda_z^{(ps)}$ may be far from sharp. We nonetheless consider the computational cost of a non-reversible subsampling MCMC to be $n(\lambda_z^{(ps)} \tau_z)^{-1}$. In Section 6.1, we discuss how the looseness of the bound may allow certain non-reversible subsampling MCMC algorithms to escape our main conclusions.
1.1. Main Bound: Informal Sketch. Consider two random datasets $Z^{(1)}, Z^{(2)}$ of size $n$ having the same distribution, and denote by $T$ a set of control variates/summary statistics allowed to depend on the entire dataset. For fixed $z, t$, let $\mathcal{A}$ be the event

$$\mathcal{A} = \{Z^{(2)} = z, Z_{1:m}^{(1)} = z_{1:m}, T(Z^{(2)}) = T(Z^{(1)}) = t\},$$

where $m = o(n)$. Let $K_{Z^{(1)}}$ be a subsampling MCMC transition kernel using subsets of the dataset $Z^{(1)}$ at each iteration with invariant measure $\pi_1$, and denote by $p_j(\cdot) = p(\cdot | Z^{(j)})$ the posterior measure under dataset $j$. Note that it need not be the case that $\pi_1 = p_1$.

One of our main results is the following. So long as there exists a coupling of $Z^{(1)}, Z^{(2)}$ such that, conditional on $\mathcal{A}$, the inequality

$$\|\pi_1 - p_1\|_{TV} \ll \|p_1 - p_2\|_{TV} \quad (1.4)$$

holds with high probability with respect to the distribution of $(Z^{(1)}, Z^{(2)})$, then subsampling MCMC can reduce overall computational cost by at most a factor of $\log(n)$. For an explanation of why using total variation in Inequality (1.4) gives a strong result, see the remark immediately following Assumption 2.2.

We refer to Inequality (1.4) as a “large fluctuation” condition. When this holds, even if we fix two data sequences that agree in their first $m \ll n$ elements and some set of statistics $T$ calculated from the entire dataset, changing only the remaining $n - m$ data points still changes the posterior “substantially.” Heuristically, it says that the invariant measure $\pi_1$ of $K_{Z^{(1)}}$ is not a better approximation to the posterior $p_1$ given data $Z^{(1)}$ than the posterior $p_2$ given some other typical dataset $Z^{(2)}$.

We can now refine our earlier trilemma in the context of (1.4). There are three possibilities, at least one of which must be true:

1. Inequality (1.4) holds (in which case the computational cost can improve by at most a factor of $\log(n)$ with subsampling); or
2. Inequality (1.4) fails with the LHS large (which suggests the algorithm is not much use for Bayesian inference); or
3. Inequality (1.4) fails with both sides small (which says that the control variates essentially determine the posterior).

It is natural to try to separately estimate the spectral gap $\lambda_z$ and per-step cost $n\tau_z^{-1}$ in Equation (1.3). This is basically the approach of many previous articles on computational efficiency of approximate MCMC algorithms, including [NDH+17]. However, we have found that it is often vastly easier to bound the product directly. To give some indication of the disparity in difficulty, using existing techniques to bound the spectral gap of a single Markov chain targeting logistic regression can be the subject of a long paper.
[JSPD19, QH19]: here we set up new techniques and give good bounds on the cost of all Markov chains targeting logistic regression.

1.2. Example: generalized linear models. To illustrate these ideas, we now give an informal corollary of our main results that applies to an important special case: using a reversible Markov chain to sample from the posterior under a generalized linear model, perhaps taking advantage of some simple control variates. In this setting, our result gives sufficient conditions under which computation time for subsampling MCMC must scale almost-linearly in the total size of the dataset, regardless of the details of the MCMC algorithm used.

We first fix a class of statistical models. Denote by \( \theta = (\beta, \sigma) \) and 
\[
p(y \mid \theta, x) = \prod_{i=1}^{n} a(y_i, \sigma) e^{\langle x_i \beta \rangle y_i - c(x_i \beta)} d(\sigma)
\] 
the usual generalized linear model (GLM) in canonical form, where \( y = (y_1, \ldots, y_n) \) and \( x = (x_1, \ldots, x_n) \) denote the response data and covariate data, respectively. Let \( z = (x, y) \) denote the full dataset. The functions \( a, c, d \) are well-known for commonly used models. For example, when the model is in canonical form, \( b \) is the identity function. For example, for logistic regression we have \( c(x) = \log(1 + x) \), \( d(\sigma) = 1 \), and \( a(y, \sigma) = 1 \).

Let \( X_1, X_2, \ldots \overset{i.i.d.}\sim \gamma \) for some distribution \( \gamma \) on a compact subset of \( \mathbb{R}^d \) with continuous density with subexponential tails satisfying the first Assumption 4.1. Fix a “true” model parameter \( \theta_0 \in \mathbb{R}^d \), and let \( Y_i \mid X_i \overset{\text{iid}}{\sim} p(\cdot \mid \theta_0, X_i) \) be drawn independently from the same regression model with parameter \( \theta_0 \) and covariates \( X_i \).\(^2\) Finally, fix some prior distribution on \( \mathbb{R}^d \) that has a smooth density with respect to Lebesgue measure and subexponential support.

Next, we define the large class of data-augmentation Markov chains that our results apply to. We consider any fixed collection \( \{K_{(x, y)}\}_{x \in \mathbb{R}^d, y \in \mathbb{R}^n} \) of reversible Markov kernels on an “augmented” state space \( \mathbb{R}^d \times \mathbb{A} \), indexed by possible data sets \( z = (x, y) \). Denote by \( \pi_z \) the stationary distribution of \( K_z \), and assume that the marginal distribution of \( \pi_z \) on \( \mathbb{R}^d \) is exactly the posterior distribution \( p(\cdot \mid Z = z) \) of the regression model (1.5).

We now give a slightly more precise definition of the quantity \( \tau_z \) in (1.3). We denote by \( \tau_z(\theta, a) \) the (random) number of steps it takes for a Markov chain driven by \( K_z \) and started at \( (\theta, a) \in \mathbb{R}^d \times \mathbb{A} \) to “use” the information.

\(^2\)We will routinely overload the notation \( p \) in this way to denote both measures and densities. The underlying dominating measure is either Lebesgue or counting measure, as appropriate.
contained in \( m \equiv (n - k - 1) \) data points, where \( k \) is the number of control variates/dimension of \( T \), beyond the information contained in \( T \). We give a formal definition of “using” data in Definition 2.8, but it is exactly what one would expect: a data point is “used” in a calculation if changing the data point changes the result of the calculation.\(^3\) Similarly, a data point is “used” beyond the knowledge of some control variates if changing the data in a way that doesn’t change the control variates changes the result of the calculation.

Let

\[
\tau_z = \inf_{\theta,a} \sup \{ r \in \mathbb{R} : \mathbb{P}[\tau_z(\theta,a) > r] \geq 1 - n^{-2} \},
\]

the time it takes to “use” many data points with high probability, from the best possible starting point.

We say that a sequence of events \( \{A_n\}_{n \in \mathbb{N}} \) holds “with extreme probability” (abbreviated w.e.p.) if \( \mathbb{P}[\{A_n \text{ i.o.}\}] = 0 \), where i.o. denotes “infinitely often.” Finally, in the result that follows, \( T \) consists of the MLE estimate of \((\beta_1, \ldots, \beta_d)\) (though our abstract results apply to virtually all commonly used control variates). We then have the following immediate corollary of Theorems 3 and 6:

**Theorem 1** (Slow mixing of Subsampling MCMC for GLMs). Under the above conditions, there exists some constant \( 0 < C < \infty \) so that the cost of \( K_Z \) satisfies

\[
\text{cost}(K_Z) \equiv \frac{n}{\tau_Z \lambda_Z} \geq C \frac{n}{\log(n)}
\]

w.e.p., where the probability is with respect to the distribution of \( Z \).

For many specific families of algorithms that have been proposed, it is straightforward to sharpen the right-hand side of this bound to \( Cn \) (see Sections 5.2 and 5.3). On the other hand, for many specific examples, the computational cost of well-tuned naive Metropolis-Hastings is \( O(n) \). When these both apply, subsampling can reduce computational cost by at most a constant factor. In Sections 5.2 and 5.3, we check that two popular subsampling algorithms really do incur this extra “logarithmic penalty” under some moderate conditions. In Section 6.3, we discuss an approach to avoiding this logarithmic penalty.

\(^3\) Of course, a specific implementation of an algorithm may access a datapoint that is not “used” in this sense. For this reason our definition may **undercount** the number of datapoints accessed by an algorithm, but it will never **overcount**. In this sense our definition is conservative, portraying subsampling algorithms in the best possible light.
While Theorem 1 is stated for specific control variates, our results hold under vastly more general conditions (see e.g. the first part of Assumption A.3). We are not aware of any fixed-size collection of sample statistics suggested in the literature that do not satisfy these conditions for most generalized linear models, nor are we aware of any general strategies for finding “good” fixed-size collections that are not adaptive. This includes e.g. [HAB17], which gives exponential convergence in $k$ for fixed $n$. In contrast, our conditions concern exponential convergence in $n$ for fixed $k$, which is much more difficult to achieve. In Section 4.2, we discuss some simple models and control variates that fail our conditions; we believe these non-examples shed some light on why our conditions hold so often for realistic examples.

We note that Theorem 1 looks quite different from most theorems in the literature on bounding the spectral gaps of Markov chains. On one hand, the result holds for any sequence of Markov chains, based only on their stationary measures and some smoothness properties. It is much more common to give bounds for a specific Markov chain with a given stationary distribution, and so in this sense our result is extremely general. On the other hand, our result is only valid with high probability for large $n$, whereas many theorems about Markov chains would hold for every finite $n$. Since our goal is to do a computational complexity analysis, this result is sufficient for our purposes.

These two oddities are closely related. It is not difficult to construct a family of Markov chains that is very efficient for one dataset $(x,y)$. Thus, we can’t hope to get a bound that holds for all datasets. However, our theorem is nearly as good: while you can “cheat” and get a good Markov chain for a specific dataset, you can’t write down a family of Markov chains that is good for typical datasets. In particular, any family of Markov chains you write down is unlikely to be good for your dataset. Thus, at a minimum one needs to “solve for” a good transition kernel $K_z$ that works for each particular dataset $z$, and of course we expect this to be computationally difficult.

1.3. Literature Review. The present paper was motivated by recent work on “online” subsampling MCMC. Surveys of the topic include [BDH17a, FBPR18], which focus on the interesting specific methods introduced in [QVK19, BFR16, PFJR16] and more generally on the important role of control variates in exact subsampling MCMC. Auxiliary-variable methods are also an important part of this literature, and “exact” subsampling MCMC was introduced in this context in [MA14]. Several papers have recently given positive theoretical results on these sorts of subsampling MCMC algorithms; see e.g. [JMMD15, RS18]. These results typically require that the approximating MCMC kernel is a uniformly good approximation of the “exact” transition kernel in a Wasserstein
or total variation metric. An upshot of the results that we present here is that one typically requires $\Omega(n)$ subsample sizes to accomplish this using a subsampling approach.

There is also a large literature on trying to understand how subsampling methods work in other algorithms used in Bayesian statistics. Our current paper most closely resembles [NDH+17], which gives qualitatively similar conclusions for the stochastic gradient Langevin algorithm (SGLA) in some settings. Although our main messages are very similar, the details of our papers are quite different. Most obviously, we deal with generic subsampling while they focus on SGLA. More subtly, we provide absolute lower bounds on the convergence rates of our algorithms, while they provide only lower bounds on some natural upper bounds on convergence rates; this meant [NDH+17] left open the small possibility that substantially faster convergence is still possible when their upper bounds are not sharp.

Most previous subsampling papers involve pre-computation of control variates or other surrogates for the target distribution. Some of these have suggested adaptive choice of control variates, as in [BDH17a] and also the author’s previous [CMPS16] amongst other places. From the point of view of this paper, we view the adaptive stages of algorithms as essentially a sophisticated way of choosing good control variates. In a somewhat related direction, there is also a literature on “preprocessing” subsampling algorithms. These algorithms usually involve extensive pre-computation; see for example [HCB16] and the references therein. This approach avoids many of the issues raised in the present paper, and we believe that it has the potential to make a large impact on Bayesian computation for popular models - especially as it becomes more integrated into MCMC techniques.

In the present paper, we have focused on GLMs and other models for which the computational complexity of “default” methods scales roughly linearly in $n$. In other situations, default methods may scale much more unfavorably in $n$, which opens the door for subsampling methods to give a much larger improvement. For example, many MCMC algorithms require repeated solution of linear systems which often has at least a quadratic cost in $n$. See e.g. [SQK+19] for a recent example of subsampling in a setting in which computational costs scale super-linearly in $n$ for naive algorithms. We leave open the possibility of analogous bounds in this setting.

Finally, recall that in discussing the third part of our trilemma, we made the following somewhat facile suggestion: if the posterior conditioned on the data is extremely close to the posterior conditioned on just the control variates, you should simply run MCMC based on the control variates and ignore the data. While we think this is good advice and applies to many articles on generalized
linear models, we point out that it is not always possible, even in the rather special case that the control variates are in fact sufficient; see [Mon15] for details in an important class of models.

1.4. Paper Guide. We introduce our notation and main assumptions in Section 2 and then state (and prove) our main theorems in Section 3. In Sections 4 and 5, we illustrate how these generic results can be applied in a broad variety of realistic settings. The first of these, Section 4, verifies that our assumptions about the target distribution and control variates hold for a variety of realistic statistical models and control variates related to GLMs. It also presents several illustrative non-examples, mostly related to control variates that are very “close” to being sufficient statistics in a sense made precise in that section. The second of these, Section 5, verifies that a variety of realistic subsampling chains satisfy the main assumptions of our theorems. It also illustrates that there is some subtlety in checking when an algorithm “uses” a datapoint, and presents a construction that gives quantitatively strong bounds for a variety of subsampling algorithms that are popular in the literature. Finally, in Section 6 we discuss the broader context of this work and highlight some important problems that are left open.

We remark here that, typically, verifying that a specific model or algorithm satisfies our assumptions with “good” constants takes some work. Of course it is not possible to give a careful study of all models and algorithms within one paper, and this leads to some conflict in the presentation of the results: we wish to have clear and simple main applications for those interested in the “big picture,” while also helping readers to verify the assumptions in their particular examples. We have chosen to resolve this conflict as follows:

- Sections 4 and 5 focus on applications to specific simple models and subsampling algorithms that are currently popular in the literature, in an effort to succinctly present a variety of concrete examples and results that are most likely to be of interest to practitioners. Most proofs from these sections are deferred to technical appendices.
- Throughout the paper, we include various short remarks on technical issues that appear when using our results, and also reference the lemmas and constructions in the appendices that can be used to resolve them for most models and algorithms that we are aware of. We believe that these technical issues are to some extent unavoidable due to the generality of the current approach and the fact that algorithms can be presented in very different forms. To contrast with the closely-related work [NDH+17]: our current paper allows for generic subsampling chains and gives lower bounds on their convergence rates, while [NDH+17] studies a specific family of subsampling
chains and gives only lower bounds on upper bounds on their convergence rates. Most of the technical difficulties come from these two differences: the first means we must have a very careful definition of when a datapoint is “used,” and the second means that we must check that posterior distributions are not “almost completely” determined by small subsamples and a collection of control variates. Appendix D gives alternative representations that can help with the first issue, Appendix A.2 gives generic bounds in random matrix theory that can help with the second issue, and Appendix E illustrates how adding carefully-constructed but “unused” control variates can help both issues.

- Finally, Appendix A begins with a short guide to our constructions. We emphasize here one important part of this guide. Most of the difficulty in checking our assumptions for new models comes from a single technical condition related to the singular values of certain random matrices. While we found this condition difficult to verify by hand, in many cases it is easy to verify by computer. We give a short algorithm for this verification in Remark A.6.

Although the paper focuses on Markov chain Monte Carlo methods, the appendices include some more general material that may be of independent interest: Appendix C includes some generic bounds on anticoncentration of random variables, which are applied in Appendix B to obtain bounds on the condition number of certain highly-structured random matrices.

2. Notation

2.1. General Notation. For measures $\nu_1, \nu_2$ on a measurable space $(\Omega, \mathcal{F})$, the total variation distance between $\nu_1, \nu_2$ is given by

$$\|\nu_1 - \nu_2\|_{TV} = \sup_{A \in \mathcal{F}} (\nu_1(A) - \nu_2(A)).$$

We denote the distribution of a random variable $X$ by $\mathcal{L}(X)$, and the distribution of $X$ conditioned on a $\sigma$-algebra $\mathcal{F}$ as $\mathcal{L}(X|\mathcal{F})$. Finally, we write $X \sim \nu$ as a shorthand for $\mathcal{L}(X) = \nu$. We overload notation to denote by $X$ both a generic random variable and, in the specific case of regression models, the (random) covariates. Similarly, we will denote by $Y$ both a generic random variable and the response in a regression model. Since these two uses of the notation occur in distinct parts of the paper, it should always be clear from context which is intended.

We always denote by $\mathcal{X}$ a general metric space, endowed with the usual completion of the Borel $\sigma$-algebra. Informally, this set represents possible
values for a data point. We always denote by $n$ an integer. Informally, this represents the number of data points.

We use the usual big-O notation frequently throughout the paper. We use the phrase “$f$ is polynomially bounded” as a shorthand for “there exists some polynomial $g$ such that $f = O(g)$,” and similarly “$f$ is polynomially bounded away from 0” for “there exists some polynomial $g$ such that $\frac{1}{f} = O(g)$.”

Finally: throughout much of this paper, we condition on measure zero events without comment. In each of these situations, the underlying random variable always has a density, and so this does not cause any technical problems.

2.2. MCMC Notation and Background. We recall some definitions related to convergence of Markov chains. The spectrum of a transition kernel $K$ is given by

$$\text{Spec}(K) = \{ \lambda \in \mathbb{C} \setminus \{0, 1\}, (K - \lambda \text{Id}) \text{ is not invertible.} \},$$

where $\text{Id}$ is the identity operator. The (absolute) spectral gap of a transition kernel $K$ is given by\(^4\)

$$\lambda(K) = 1 - \sup\{ |\lambda| : \lambda \in \text{Spec}(K) \}.$$  \hspace{1cm} (2.1)

The absolute spectral gap is closely related to the convergence rate of a Markov chain. When the spectrum $\text{Spec}(K) \subset [0, 1]$ is nonnegative, it is well-known that the spectral gap of a reversible kernel is very tightly related to the asymptotic variance of the associated ergodic averages for worst-case functions, a result which is summarized in (1.2). In the context of the main results in this paper, we can think of this relationship as also holding for reversible kernels with a negative spectrum, as made formal in the following remark.

Remark 2.1. Consider a reversible kernel $K$, and let $K' = \frac{1}{2}(K + \text{Id})$ be the associated “half-lazy” kernel. We note two important facts about $K'$: it always has nonnegative spectrum

$$\text{Spec}(K') = \left\{ \frac{1}{2}(1 + \lambda) : \lambda \in \text{Spec}(K) \right\} \subset [0, 1],$$

and its asymptotic variance in (1.2) differs by at most a factor of 2 relative to $K$. Putting these together, the asymptotic variance of the ergodic averages associated with $K$ are very tightly linked to the spectral gap of its $\frac{1}{2}$-lazy kernel.

\(^4\)Above we have denoted the spectral gap, pseudo spectral gap, and other quantities with subscript $z$ to emphasize their dependence on the data. Elsewhere, we wish to emphasize dependence on the Markov transition kernel, and instead write e.g. $\lambda(K)$ in lieu of $\lambda_z$. This notational variation is to make statements of theorems clearer; $\lambda$ always represents the spectral gap, $\lambda^{(ps)}$ the pseudo spectral gap, and $\tau$ the number of steps necessary to use all of the data points.
Furthermore, whenever $K$ satisfies the assumptions of our main theorems, the half-lazy version $K'$ does as well. Thus, when considering a given kernel $K$, we can always apply our results to $K'$ and obtain as an immediate corollary essentially the same conclusion for $K$ itself, losing at most a factor of 2.

For this reason, issues of positivity of the spectrum for reversible kernels can be safely ignored throughout the remainder of the paper - we can always apply our results to an associated kernel with nonnegative spectrum and then draw conclusions for the original kernel of interest.

This relationship is more complicated for nonreversible kernels. One of the strongest results in this direction that we are aware of is stated in terms of the pseudo-spectral gap defined in \cite{paulin2015spectral}:

$$\lambda_{ps}(K) = \sup_{s \in \mathbb{N}} \frac{\lambda(K^s)}{s}.$$  

See e.g. Theorems 3.5 and 3.7 of \cite{paulin2015spectral} for the relationship between (pseudo-) spectral gap and asymptotic variance of an associated MCMC estimator. Although we focus here on the pseudo-spectral gap, we suspect that a similar theory could be developed for other notions of contractivity for nonreversible chains (e.g. the $V$-norm used in \cite{jones2004} and \cite{karlin2012}).

We will use the following bound, which summarizes Propositions 3.3 and 3.4 of \cite{paulin2015spectral}, quite heavily:

**Theorem 2** (Warm Start Bounds: $L^2$ to $L^1$ Convergence). For a reversible Markov chain $K$ with spectral gap $\lambda(K)$ and stationary measure $\pi$, we have for any measure $\mu$ and time $t \in \mathbb{N}$

$$\|\mu K^t - \pi\|_{TV} \leq \frac{1}{2} \sqrt{\int_{\Theta} \frac{d\mu}{d\pi}(\theta) \pi(\theta) d\theta (1 - \lambda(K))^t}. \quad (2.2)$$

If $K$ is non-reversible, let $\lambda_{ps}(K)$ be its pseudospectral gap. Then

$$\|\mu K^t - \pi\|_{TV} \leq \frac{1}{2} \sqrt{\int_{\Theta} \frac{d\mu}{d\pi}(\theta) \pi(\theta) d\theta (1 - \lambda_{ps}(K))^{t-(1-\lambda_{ps}(K))^{-1}}. \quad (2.3)$$

For these bounds to be useful, the Radon-Nikodym derivative $d\mu/d\pi$ must have bounded $L^1(\pi)$ norm. This is a form of “warm start” condition. Note that although Lemma A.1 shows that the mixing times from a “warm-start” measure $\mu$ can be bounded by $\lambda_{ps}$ for a non-reversible kernel in much the same way as by $\lambda$ for a reversible kernel, the bound in (1.2) is not sharp with $\lambda$ replaced by $\lambda_{ps}$ when $K$ is not reversible. Nonetheless, for most of the remainder of the paper, we will think of $\lambda_{ps}$ and $\tau_{rel}$ more or less interchangeably, and
take them both to be measures of the computational cost of MCMC related to the variance of ergodic averages.

2.3. Illustrative Examples: What Can We Hope For? We note that several papers on subsampling methods (see e.g. Section 5 of [FBPR18]) have discussed the possibility of developing algorithms whose computational cost scales “sublinearly” in the number of data points. We found this language mildly confusing when we first encountered it, and one goal of the present paper is to clarify it. Thus, before giving technical details, we consider a simpler question: how much improvement can we hope for with subsampling methods? This section focuses on simple examples and can easily be skipped by readers interested only in the generic results.

We begin by observing that a typical size-$m_n = o(n)$ subsample of a size-$n$ dataset cannot (generally) capture all of the information in the original dataset. Consider the simple 2-level hierarchical model:

\[ \mu \sim \mathcal{N}(0, 1) \]
\[ Y_1, \ldots, Y_n \sim \mathcal{N}(\mu, 1), \]

where $\mu$ is an unobserved hyperparameter and $Y_1, \ldots, Y_n$ is the observed data. If $m_n = o(n)$ is the size of a small subsample chosen uniformly at random, then it is straightforward to show that the posteriors associated with the full sample and the subsample are very far apart:

\[ \lim_{n \to \infty} \| p(\cdot \mid Y_1, \ldots, Y_n) - p(\cdot \mid Y_1, \ldots, Y_{m_n}) \|_{TV} = 1. \]  

(2.5)

Rescaling to e.g. force the variances to match does not help for typical subsamples. For all fixed $\epsilon > 0$, we still have

\[ \limsup_{n \to \infty} \mathbb{P} \left[ \left\| p(\cdot \mid Y_1, \ldots, Y_n) - p(\cdot \mid Y_{\sigma(1)}, \ldots, Y_{\sigma(m_n)}) \right\|_{TV} < 1 - \epsilon \right] = 0 \]  

(2.6)

where $\sigma \sim \text{Unif}(S_n)$ is a random permutation and $S_n$ is the symmetric group. Thus, even in this toy problem, posterior approximations based on subsamples are not close to the full posterior in the total variation metric when the number of data points used in the subsample grows more slowly than the total sample size. Of course, this is the only setting in which computational costs per iteration are lower for subsampling.

These calculations are all well-known, and this not what is usually intended by the phrase “sublinear cost.” Instead of considering algorithms that literally use a subsample that grows sublinearly with the size $n$ of the dataset, we should consider algorithms that are allowed to take a small subsample of size $m_n = o(n)$ and also use some computationally-cheap summary statistics of the entire dataset, such as the MLE. In the context of computational work,
these summary statistics are also often referred to as “control variates,” and we will use the two terms interchangeably. The question then becomes: is it possible to develop an exact algorithm which scales sublinearly in the size $m$ of the subsample if you take advantage of summary statistics? The possibility of such an algorithm is not ruled out by the simple calculation above, and indeed it is often possible to get very good estimates using a few carefully-chosen control variates and a very small subsample. It may even be possible for the limit corresponding to Equation (2.5) to approach 0 rather than approaching 1. For example, as is nicely illustrated in [CB18], specific subsamples can approximate the full dataset very well. In the present context, the approach of [CB18] suggests that for appropriately-chosen metrics $d$,

$$\inf_{\sigma \in S_n} d(p(\cdot \mid Y_1, \ldots, Y_n), p(\cdot \mid Y_{\sigma(1)}, \ldots, Y_{\sigma(m_n)}) \simeq (1 - \alpha)^{m_n}$$

for some $\alpha > 0$ and all $n, m_n$ sufficiently large, for typical datasets.

The perhaps-suprising conclusion of our paper is that it is often not possible to use subsampling MCMC to quickly refine initial estimates, whether they are good or not. This point is rather subtle: it suggests that very good estimates obtained by subsampling MCMC and careful use of control variates are largely due to the careful use of control variates, with the further MCMC steps improving this initial estimate very slowly as the size of the subsample increases.

To complete this discussion, we consider the reverse question: how quickly does the computational complexity of naive MCMC grow with the size $n$ of the data set? In the simple example considered in Equation (2.4), it is straightforward to check that the spectral gap of a Metropolis-Hastings chain with appropriately-scaled proposals (e.g. proposal kernel $Q_n(x, \cdot) = \text{Unif}([x - n^{-1/2}, x + n^{-1/2}])$) does not go to 0 as $n$ goes to infinity. Thus, the cost of naive Metropolis-Hastings is $O(n)$, and the standard MCMC CLT in (1.1) tells us that it is possible to obtain an MCMC estimate with a desired fixed standard deviation $\epsilon > 0$ by accessing a data point a total of $O(n\epsilon^{-2})$ times. This non-decay of spectral gap is fairly common in low-dimensional applied problems, and there is some evidence that it also occurs in realistic high-dimensional problems (see e.g. the recent papers [YR17], [QH17]).

To summarize: in even the simplest example, it is necessary to view $\Omega(n)$ data points to obtain “good” estimates. Conversely, for a wide variety of problems it is possible to obtain estimates with error less than any desired constant $\epsilon > 0$ using standard – i.e. non-subsampling based – methods while viewing only $O(n\epsilon^{-2})$ data points. Thus, the entire theoretical question is to determine if the dependence on the accuracy parameter $\epsilon$ can be improved.
As mentioned above, this discussion avoids several important practical issues. For example, on real computers, the computational cost of accessing data does not depend linearly on the amount of data accessed—there are very large discontinuities as different data buffers are used. This is largely out of the scope of the current paper, but we give some discussion in Section 6.

2.4. Notation for Subsampling MCMC and Main Assumptions. We continue more formally, introducing some notation that will be used throughout the remainder of Sections 2 and 3. As these assumptions are likely unfamiliar to the reader, we give some guidance on how to interpret them, verify them, and think about possible non-examples.

We denote by $Z^{(1)} = (Z_{1}^{(1)}, ..., Z_{n}^{(1)}) \in \mathbb{Z}^n$ a random dataset, and let $Z^{(2)} = (Z_{1}^{(2)}, ..., Z_{n}^{(2)}) \in \mathbb{Z}^n$ be another random variable with the same distribution. We do not yet make any specific assumptions about the joint distribution of $Z^{(1)}, Z^{(2)}$, or about their (in)dependence. For $k \in \mathbb{N}$, denote by $T_{1}, ..., T_{k}$ some maps with domain $\mathbb{Z}^n$, which we refer to as control variates. Let $T = (T_{1}, ..., T_{k})$ be the composite map. The control variates $T_{1}, ..., T_{k}$ will contain all information that is computed prior to running MCMC, and may include "typical" control variates such as a sample mean and variance, as well as any global information used to improve computational efficiency (e.g. the "upper and lower bound" functions $B_{n}, L_{n}$ used in [MA14]). Finally, denote by $E \subset \mathbb{Z}^n$ a collection of "good" datasets and $T(E) \subset E^*$ the associated collection of "good" summary statistics. We will make precise what is meant by "good" in this context shortly.

Most assumptions in this section are stated for fixed data size $n$ when this makes sense. Later, we will sometimes consider sequences indexed by the size $n$ of the dataset. In this situation, we will use the superscript $(n)$ to denote any sequence that satisfies the associated assumption for all fixed $n > N_0$ sufficiently large. In this case, any constants $c_i, C_i$ appearing in the assumptions will always be independent of $n$.

Our main definition is the following large fluctuations condition:

**Assumption 2.2 (Large Fluctuations).** Fix $m \in \mathbb{N}$ and $0 \leq c_1, C_1 < \infty$. For $z \in E$ and $t \in E^*$, let $\mathcal{A} = \mathcal{A}(z)$ be the event

$$\mathcal{A} = \{ Z^{(2)} = z, Z_{1:m}^{(1)} = z_{1:m}, T(Z^{(2)}) = T(Z^{(1)}) = t \}. \quad (2.7)$$

We say that the posterior $p$ exhibits $(c_1, C_1)$-large fluctuations on $E$ for subsamples of size $m$ if there exists a coupling of $Z^{(1)}, Z^{(2)}$ such that, conditional on $\mathcal{A}$,

$$\| p(\cdot | Z^{(2)}) - p(\cdot | Z^{(1)}) \|_{TV} \geq C_1 n^{-c_1} \quad (2.8)$$

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Although it is not emphasized in the notation, we note that this condition implicitly depends on the data-generating process for \(Z^{(2)}, Z^{(1)}\). When we don’t need to emphasize the constants \(c_1, C_1\), we drop them and call this the large fluctuation condition.

The choice of the total variation metric in Assumption 2.2 is very important. Notice that the stronger the metric used in Assumption 2.2, the weaker the assumption, since it is “easier” for two distributions to be far away in a strong metric than in a weak one. If total variation were replaced by a weaker metric, such as the Prokhorov metric, the assumption would hold for far fewer cases of interest.

Assumption 2.2 can be paraphrased as saying: even after seeing a subsample of size \(m\) and the values of the summary statistics, there is still uncertainty about the posterior distribution (as measured by the TV norm). Assumption 2.2 does not hold for all statistical models, and indeed it fails for many “textbook” distributions. In particular, it certainly fails if \(T\) is a sufficient statistic. However, we expect the assumption to hold for essentially any distribution that one would target using MCMC. Indeed, if it fails, we think of \(T_1, \ldots, T_k\) as quantitatively almost indistinguishable from being sufficient statistics. In these special cases it is typically not worthwhile to use MCMC based on the full dataset at all (though again see [Mon15] for some situations where this is not true).

We will establish Assumption 2.2 in a simple realistic situation in Section 4, and we give more general and very weak sufficient conditions in Appendix A. Section 4 also includes a nontrivial example where the assumption fails: this is a model that doesn’t have any exactly sufficient statistics, but which has statistics that behave very much like sufficient statistics in some regions of the parameter space. As we will see in Section A, showing that this assumption holds is closely related to proving an “anti-concentration” result; see e.g. [Cha19] or Section 1.2 of [RV08] for generic techniques that are useful in proving such an anti-concentration result.

Remark 2.3 (Why Do We Need Sets \(E, E^*\) ?). Note that Assumption 2.2 will often fail if we take \(E = Z\). To see this, consider a very light-tailed distribution \(p\) and the test statistic \(T(Z) = \frac{1}{n} \sum_{i=1}^{n} z_i\). As \(t\) and \(n\) become very large, conditioning on the event \(\{T(Z) = t\}\) becomes more and more similar to conditioning on the event that \(z_i \approx t\) for all \(1 \leq i \leq n\). If \(p\) is sufficiently light-tailed, the error in the approximate equality \(z_1 \approx t\) can go to 0 very quickly. In effect, this means that the average \(T(Z)\) almost determines the full vector \(Z\) and thus acts (quantitatively) as a sufficient statistic. See
Section 4.2 for a detailed example which illustrates this general phenomenon.
In practice, we expect it to be easy to find a set \( E \) that contains all \( n \) data points with high probability, while remaining fairly small. For example, if \( Z_1^{(1)}, \ldots, Z_n^{(1)} \sim \mathcal{N}(0, 1) \), we might choose e.g. \( E = (-10\sqrt{\log(n)}, 10\sqrt{\log(n)}) \).
We do not expect this restriction to be a large obstacle to the analysis of realistic algorithms and datasets - it simply means excluding datasets that are extremely implausible under the model of interest.

We also assume that it is possible to build “warm starts” using only a few summary statistics:

**Assumption 2.4 (Warm Starts).** There exist constants \( 0 \leq c_2, C_2 < \infty \) and a family of measures \( \{\mu_t\}_{t \in E^*} \) with densities \( \rho_t \) so that

\[
\sup_{Z : T(Z) = t} \max_{\theta \in \Theta} \frac{\rho_t(\theta)}{p(\theta \mid Z)} \leq C_2 n^{c_2} \tag{2.9}
\]

w.e.p.

Since we allow the ratio to become quite large as \( n \) grows, very simple warm starts (such as the uniform distribution on a ball of radius \( n^{-2} \) around the MLE) work well in our context. While we mention using a ball around the MLE because our examples are mainly generalized linear models, in which a unique MLE exists, in fact the warm start condition is much weaker than that. For example, if the target has polynomially (in \( n \)) many modes and a density satisfying some mild smoothness conditions, it is still possible to construct a warm start satisfying (2.9). See Appendix A.1 for details and a discussion of improved constants.

**Remark 2.5 (Extra Control Variates and Verifying Assumptions).** At first glance, it seems that Assumption 2.4 must fail for algorithms that don’t use any control variates - it is typically impossible to satisfy Inequality (2.9) uniformly over all datasets. Fortunately, this is usually easy to fix by adding in additional “unused” control variates. More precisely: in our current setup, the collection of control variates \( T \) must include all control variates that the Markov chain actually accesses when it is implemented. However, our formal setup also allows us to add any number of additional control variates to this collection, even if they are not used to construct \( K \).

These “extra” control variates will not influence the algorithm and need not be computationally tractable. However, well-chosen extra control variates can sometimes allow us to achieve conditions (2.7) and (2.9) simultaneously. In other words, when verifying our assumptions, we are always allowed to simply throw in more control variates than the algorithm actually takes advantage
of - the results will still stand. Theorem A.1 implies that adding the MLE is sufficient to obtain Assumption 2.4 for a wide variety of models.

We assume that the set $E$ has very high probability:

**Assumption 2.6** (Good Set Has High Probability). Assume that the event

$$\{Z^{(1)} \in E\}$$

holds w.e.p.

We have had no difficulty in verifying this assumption for e.g. generalized linear models with reasonable data generation models for covariates.

Next, we give a precise notion of a “subsampling chain.” Intuitively, we simply wish to measure which data points were “actually” used in the first steps of a Markov chain. However, stating this precisely requires us to be careful. The main difficulty is that many existing subsampling algorithms, such as [MA14], are written in a form that assumes the computer has access to the entire dataset at every step. By being somewhat careful with our definitions, we can say in a precise way that these algorithms don’t “actually” use all of the data at each step.

Consider a family $\{K^*_z\}_{z \in E}$ of ergodic Markov transition kernels on state space $\Theta \times \mathcal{A}$ with stationary distributions $\pi_z$. This family consists of the subsampling MCMC kernels under consideration. We denote by $\mathcal{P} : \Theta \times \mathcal{A} \mapsto \Theta$ the projection map $\mathcal{P}(\theta, a) = \theta$. We assume that there exists a function $F : [0, 1] \times \mathbb{Z}^n \times (\Theta \times \mathcal{A}) \times \mathbb{N} \mapsto \Theta$ called the forward map so that, for $U$ sampled according to $U \sim \text{Unif}([0, 1])$ and $z, \theta, s$ viewed as fixed, we have

$$F(U, z, \theta, s) \sim K^*_z(\theta, \cdot).$$

The assumption that such a map $F$ exists is extremely weak. To our knowledge, all implementations of MCMC algorithms on computers involve the construction of such a function, called a random mapping representation. See e.g. [JKR15] and the literature cited therein for various general sufficient conditions.

While $s$ has been an arbitrary integer up to this point, in interpreting the results that follow it is useful to think of $s$ as approximately equal to $\tau_z$ wherever it appears. In practice, we will choose a sequence of values of $s$ that satisfies this condition.

**Remark 2.7** (Why Augment $\Theta$?). We allow for an augmented state space so that our result applies directly to data-augmentation algorithms such as [MA14], and also to algorithms such as sequential Monte Carlo (SMC) that can be written as high-dimensional Markov chains.
We take note of the following obvious objection to the main thrust of this article: there could be a data-augmentation chain that mixes slowly, but for which the relevant projection mixes quite quickly. Such a chain would satisfy our assumptions, but still produce small-variance estimates for the quantities of interest. In practice this seems fairly unlikely to us, and there are various well-known conditions under which a full data-augmentation chain mixes at the same rate as some of its projections (see e.g. [LWK94]). We point out in Section 5 that several specific subsampling algorithms in the literature have this property, and so we avoid the objection for these specific algorithms.

In other situations, we might not know a priori that the projection mixes at the same rate as the full chain. In these cases, one could use function-specific mixing bounds (as in e.g. [RRJW18]) in place of the full-chain mixing bounds in Lemma 2 to obtain similar estimates. Doing so is beyond the scope of the current paper.

We now define a collection of functions $f_{u,\theta,s}$ indexed by $u \in [0,1]$, $\theta \in \Theta$ and $s \in \mathbb{N}$ that maps the data to $\Theta \times A$. The purpose of this function is to make precise for which of the data points in $z$ the forward map $F$ is non-constant.

**Definition 2.8** (Subsampling Chain). Fix $u \in [0,1]$, $\theta \in \Theta \times A$ and $s \in \mathbb{N}$, so that

$$f_{u,\theta,s}(\cdot) \equiv F(u,\cdot,\theta,s) : Z^n \mapsto \Theta \times A$$

can be viewed as a function from the data $z \in E$ to the parameter $\tilde{\theta} \in \Theta \times A$. Call a set $Z^* \subseteq \{1,\ldots,n\}$ stable if $f_{u,\theta,s}(z)$ is constant $z_j$ for every $j \in Z^*$ and every $z \in E$. Let $Z_{\text{sub}} = Z_{\text{sub}}(u,\theta,s)$ be any $U,\theta$-measurable map that selects exactly one element from the collection of all stable sets.

**Remark 2.9.** There is an important special case where it is very easy to write down a reasonable map. If your algorithm explicitly selects a subset $S_t = S_t(U,\theta)$ of the data points at every time $t$, one can just take $Z_{\text{sub}}(U,\theta,s) = (\bigcup_{t \leq s} S_t)^c$. This special case includes most algorithms in the literature and our generic algorithms in Section 5. We allow the added generality of Definition 2.8 because, in some situations, this construction may give suboptimal bounds and it may not be obvious how to construct $S_t(U,\theta)$ at all.

Notice that $Z_{\text{sub}}(U,\theta,s)$ is a random variable, and its distribution will determine the value of the constant $\tau_z$ that appears in (1.3) for any $z \in E$. In the remainder of the paper, we will view the summary statistics $T(Z) = t$ as fixed and define

$$R = R(n,t) \equiv \{z \in E : T(z) = t\}. \quad (2.11)$$
If a subsampling algorithm is to have any advantage over a default full-sample algorithm, \(|Z_{\text{sub}}|\) must typically be comparable to \(n\). We formalize this in the following assumption:

**Assumption 2.10 (Small Dependence).** Let \(c_1\) be as in Assumption 2.2. For \(n \in \mathbb{N}\) and \(t^{(n)} \in \mathbb{R}^{kd}\), let \(R \subset \mathbb{Z}^n\) be as in Equation (2.11), consider the restricted family of Markov chains \(\{K_Z\}_{Z \in R}\), and let \(U \sim \text{Unif}([0, 1])\). We say that the integer-valued sequences \(\{m^{(n)}\}\), \(\{s^{(n)}\}\) and the sequence of sets \(\{E^{(n)}\}\) exhibit small dependence if the random subsets \(Z^{(n)}_{\text{sub}} = Z_{\text{sub}}(U, \theta, s^{(n)})\) from Definition 2.8 satisfy

\[
Z^{(n)}_{\text{sub}} \supset \{m^{(n)}, \ldots, n\} \quad (2.12)
\]

together w.e.p., uniformly in the choice of \(\theta \in \Theta \times A\). Note that the randomness in this expression is induced by \(U \sim \text{Uniform}([0, 1])\) — i.e. it relates to the randomness of the Markov chain.

Recall that in applying our results, one should think of \(s^{(n)} \approx \tau_z\). Of course this also means that in practice, \(m^{(n)}\) and \(s^{(n)}\) can’t be chosen independently.

**Remark 2.11 (Subsamplers with Unbounded Sample Size).** Assumption 2.10 is the only assumption that must be checked on a per-algorithm basis. It is clear that the assumption is satisfied for some choice of parameters; however, to obtain good bounds on the spectral gap, one should check that it is satisfied for some specific sequence \(m^{(n)}, s^{(n)}\) for which \(s^{(n)}\) is reasonably large.

We briefly outline the main difficulties in verifying that this assumption holds for large \(s^{(n)}\), and where they are addressed in the paper:

- In simple algorithms, one can use standard concentration inequalities to quickly verify that a large value of \(s^{(n)}\) is possible. See Section 5 for examples.
- In many algorithms, the possible values of \(s^{(n)}\) depend heavily on the choice of forward-mapping representation of the algorithm. See Section 5 again for an example of a simple algorithm with a very poor value of \(s^{(n)}\) under one naive forward-mapping representation, as well as a simple reparameterization trick that gives an optimal value.
- In some algorithms, the best value of \(s^{(n)}\) may depend heavily on the control variates used. See Appendix E for details on a simple construction that can partially alleviate this problem.

We also have a pair of alternatives to Assumptions 2.2 and 2.10. We find that these can give much sharper results for certain algorithms — see Section 5 for applications of these new assumptions and a quick discussion of why they are useful. Our alternative to Assumption 2.2 is:
Assumption 2.12 (Large Fluctuations (Alternative)). Fix notation as in Assumptions 2.2 and 2.10. Define the random time
\[ S = \max \left\{ t : \left| Z^{(n)}_{\text{sub}}(U, \theta, t) \right| \geq n - m^{(n)} \right\} \]
and let \( I = Z^{(n)}_{\text{sub}}(U, \theta, S) \). This assumption is as Assumption 2.2, with Equation (2.7) replaced by:
\[ A = \{ Z^{(2)} = z, Z^{(1)}_{I} = z, T(Z^{(2)}) = T(Z^{(1)}) = t \} . \]
Our alternative to Assumption 2.10 is:
Assumption 2.13 (Small Dependence (Alternative)). As Assumption 2.10, with Equation (2.12) replaced by:
\[ |Z^{(n)}_{\text{sub}}| \geq n - m^{(n)}. \]

3. Main Results

We now state and prove our main abstract results, with all notation carried over from Section 2. All results in this section hold when both Assumptions 2.2 and 2.10 are replaced by their alternatives 2.12 and 2.13, with essentially identical proofs.

Our first result applies to reversible Markov chains, including data-augmentation chains.

**Theorem 3.** Let Assumption 2.2 be satisfied for \((Z^{(1)}, Z^{(2)}) = \{(Z^{(1,n)}, Z^{(2,n)})\}_{n \in \mathbb{N}}\) with the independence coupling, a sequence of integers \(\{m^{(n)}\}\), and sequence of good sets \(\{E^{(n)}\}_{n \in \mathbb{N}}\) satisfying Assumption 2.6. Let Assumptions 2.4 and 2.10 also be satisfied, for the same sequence \(\{m^{(n)}\}\) and another sequence of integers \(\{s^{(n)}\}\). Finally, let \(\lambda_{Z}\) be the spectral gap of \(K_{Z}\). If \(K_{Z}\) is reversible for all \(Z \in E\), then
\[ -\log(1 - \lambda_{Z}) \leq \frac{c_{1} + c_{2}}{2s^{(n)}} \log(n) \]
holds w.e.p.

Before giving the proof, we relate the notation in this theorem back to our informal notion of computational cost in Equation (1.3). The “time to use almost all of the data” that appears as \(\tau_{z}\) in (1.3) is formalized here as the sequence of integers \(\{s^{(n)}\}\); the relaxation time \(\tau_{\text{rel}}\) that appears in (1.3) is
the reciprocal of the spectral gap $\lambda_Z$ that appears here. Thus, this theorem is saying that

$$\text{cost}(K_Z) \gtrsim \frac{n}{\log(n)}$$

holds w.e.p.

**Proof.** The proof proceeds by decoupling. We initialize two Markov chains, driven by $K_{Z(1)}$ and $K_{Z(2)}$, at the same point and then bound their decoupling time.

Let $\rho$ be the “warm” starting distribution guaranteed to exist by Assumption 2.4. Sample $\theta \sim \rho$ and $U \sim \text{Unif}([0, 1])$, and let $Z_{\text{sub}} = Z_{\text{sub}}(U, \theta, s)$ be the random set described in Definition 2.8. Let $\mathcal{A}$ be as in (2.7) and let $\mathcal{B}$ be the event that $Z_{\text{sub}} \supset \{m, \ldots, n\}$. We note that, on the event $\mathcal{B} \cap \mathcal{A}$,

$$F(U, Z^{(1)}, \theta, s) = F(U, Z^{(2)}, \theta, s).$$

By our assumptions, $\mathcal{B} \cap \mathcal{A}$ holds w.e.p., so there exists a sequence $\{\omega_n\}$ with $\lim_{n \to \infty} \omega_n = 0$ such that

$$\| (\rho K_{Z(1)}^s)(P^{-1}(\cdot)) - (\rho K_{Z(2)}^s)(P^{-1}(\cdot)) \|_{\text{TV}} \leq \omega_n n^{-c_1} \quad (3.1)$$

holds w.e.p. On the other hand, by Assumption 2.2,

$$\| \pi_{Z(1)}^{-1}(\cdot) - \pi_{Z(2)}^{-1}(\cdot) \|_{\text{TV}} \geq C_1 n^{-c_1} \quad (3.2)$$

holds w.e.p. as well. Finally, by Theorem 2 and Assumption 2.4,

$$\| (\rho K_{Z(1)}^s)(P^{-1}(\cdot)) - \pi_{Z(1)}^{-1}(\cdot) \|_{\text{TV}} \leq C_2 n^{c_2} (1 - \lambda_{Z(1)})^s \quad (3.3)$$

and

$$\| (\rho K_{Z(2)}^s)(P^{-1}(\cdot)) - \pi_{Z(2)}^{-1}(\cdot) \|_{\text{TV}} \leq C_2 n^{c_2} (1 - \lambda_{Z(2)})^s.$$

Applying Inequalities (3.1), (3.2) and (3.3), we have w.e.p.

$$C_2 n^{c_2} (1 - \lambda_{Z(1)})^s \geq \| (\rho K_{Z(1)}^s)(P^{-1}(\cdot)) - \pi_{Z(1)}^{-1}(\cdot) \|_{\text{TV}}$$

$$\geq \| \pi_{Z(1)}^{-1}(\cdot) - \pi_{Z(2)}^{-1}(\cdot) \|_{\text{TV}} - \| (\rho K_{Z(2)}^s)(P^{-1}(\cdot)) - \pi_{Z(2)}^{-1}(\cdot) \|_{\text{TV}}$$

$$\geq \| \rho K_{Z(1)}^s(P^{-1}(\cdot)) - \pi_{Z(1)}^{-1}(\cdot) \|_{\text{TV}} - \| (\rho K_{Z(2)}^s)(P^{-1}(\cdot)) - \pi_{Z(2)}^{-1}(\cdot) \|_{\text{TV}}$$

$$\geq (C_1 - \omega_n) n^{-c_1} - C_2 n^{c_2} (1 - \lambda_{Z(2)})^s.$$

Rearranging and recalling that $\lambda_{Z(1)}, \lambda_{Z(2)}$ are independent and have the same distribution, we have

$$(1 - \lambda_{Z(1)})^s \geq \frac{1}{2} C_2^{-1} C_1 n^{-c_1 - c_2}.$$
holds w.e.p. Note that in obtaining the above display, we used the fact that if two independent, nonnegative random variables $X, Y$ with the same distribution satisfy $X + Y > A$ w.e.p., then $X > A/2$ w.e.p. This immediately implies the result.

For nonreversible chains, we have essentially the same result:

**Theorem 4.** With notation as in Theorem 3, and letting $\lambda_{(Z, ps)}$ be the pseudo-spectral gap of $K_Z$,

$$ - \log(1 - \lambda_{(Z, ps)}) \leq \frac{c_1 + c_2}{68(n)} \log(n) $$

holds w.e.p.

**Proof.** The proof is identical to the proof of Theorem 3, replacing the reference to Inequality (2.2) with a reference to Inequality (2.3).

The previous results give conditions for slow mixing under the assumption that the marginal distribution of $\pi_Z$ is exactly $p(\cdot | Z)$. However, similar results hold as long as $\pi_Z$ gives a much better approximation of $p(\cdot | Z)$ than can be obtained from the summary statistics alone:

**Theorem 5.** Set notation as in Theorem 3, but replace Inequality (2.8) of Assumption 2.2 with the condition that

$$ \| \pi_{Z(1)}(P^{-1}(\cdot)) - \pi_{Z(2)}(P^{-1}(\cdot)) \|_{TV} \geq C_1 n^{-c_1} $$

holds w.e.p. That is, the $\theta$-marginals of the invariant measures are at least $C_1 n^{-c_1}$ apart in total variation w.e.p. Then the conclusion of Theorem 3 holds as stated.

**Proof.** The proof is identical to the proof of Theorem 3, with one substitution: Inequality (3.2) is justified by an appeal to Inequality (3.4) rather than an appeal to Inequality (2.8) of Assumption 2.2.

This result is useful in analyzing “approximate” chains, such as those studied in [QVK19]. Roughly speaking, Theorem 3 says that exact subsampling MCMC cannot greatly speed up mixing, while Theorem 5 says that approximate MCMC can only greatly speed up mixing if the bias introduced by using the approximation is large (in the sense of Inequality (3.4)).
4. Examples: Targets and Control Variates

In Section 4.1 we give our main example, showing that our conditions (2.7) and (2.9) hold for logistic regression. In Section 4.2, we discuss two “non-examples”: a model with sufficient statistics, and another model with summary statistics that are “almost” sufficient in a sense that we make precise. All substantial proofs are deferred to Appendix A.

4.1. Generalized linear models. We check that our results apply to generalized linear models. Denote by

\[ p(\beta \mid x, y) = M(y, x)^{-1} p_0(\beta) \prod_{i=1}^{n} a(y_i, \sigma) e^{\frac{(x_i \beta) y_i - c(x_i \beta)}{d(\sigma)}} \]

the usual overdispersed generalized linear model on \( \mathbb{R}^d \) with some smooth prior \( p_0(\beta) \) and the dispersion parameter \( \sigma \) known. Define the maps \( T_1^{(n)}, \ldots, T_d^{(n)} \) to be the maps that return the components of the sample MLE for \( \beta \), and let \( T_{d+1}^{(n)}, \ldots, T_k^{(n)} : \mathbb{R}^{dn_1} \rightarrow \mathbb{R} \) be any further collection of smooth maps.

Let \( X_1, X_2, \ldots \sim i.i.d. \gamma \) for some distribution \( \gamma \) on \( \mathbb{R}^d \) satisfying the following fairly mild assumption:

**Assumption 4.1.** We assume that

1. \( \gamma \) is supported on a compact set \( I \subset \mathbb{R}^d \) containing the unit ball, and furthermore that it has a smooth density \( g \) with respect to Lebesgue measure. For \( n \in \mathbb{N} \), define \( g_n(x_1, \ldots, x_n) = \prod_{i=1}^{n} g(x_i) \) to be the product density; we assume there exist constants \( 0 < d_1 < \infty \), \( 1 < d_2 < \infty \) so that

\[ \sup_{x \in I^n} \sup_{\|x - \tilde{x}\| \leq n^{-d_1}} \left| \frac{g_n(x)}{g_n(\tilde{x})} - 1 \right| \leq n^{-d_2}. \]  

(4.1)

2. Denote by \( \gamma_{n,Y} \) the conditional distribution of \( X \) given response variable \( Y \), and \( g_{n,Y} \) its density. Assume that w.e.p. Inequality (4.1) also holds with \( g_n \) replaced by \( g_{n,Y} \).

Slightly abusing notation, we say that a deterministic \( y \) satisfies the second part of this assumption if (4.1) holds with \( g_n \) replaced by \( g_{n,Y} \).

Fix \( \beta_0 \in \mathbb{R}^d \), and let \( Y_i \sim p(\cdot \mid \beta_0, X_i) \) be drawn from the logistic regression model with parameter \( \beta_0 \) and covariates \( X_i \). Under this assumption on the prior and \( \gamma \), and with data generated from a true GLM with parameter \( \beta \), the MLE \( \hat{\beta} \) converges to \( \beta_0 \) almost surely (see e.g. Theorem 2 of [FK+85]).

\(^5\)In this statement we view \( \gamma_{n,Y} \) as a random measure, depending on \( Y \).
The main result of this section is:

**Theorem 6.** The logistic regression model with control variates $T_1, \ldots, T_d$, $\gamma$ satisfying Assumption 4.1 and prior $p_0$ being smooth with subexponential tails, satisfies Assumptions 2.2, 2.6 and 2.4 (with constants $c_i, C_i$ that do not depend on $n$).

The proof of Theorem 6 is deferred to Appendix A.

**Remark 4.2** (Verifying Other Control Variates). We give a quick guide to verifying the conclusion of Theorem 6 for other control variates. Following our proof of the theorem, the same conclusion holds with $T_1, \ldots, T_d$ augmented by any collection of control variates $T_{d+1}, \ldots, T_k$, as long as the first condition in Assumption A.3 is satisfied. Verifying this condition is the most difficult part of the proof of Theorem 6, as it requires us to analyze the singular values of a random matrix with highly dependent entries. In the appendix we give two generic results that allow us to verify this condition in a variety of important special cases:

1. In Appendix E, we define a special collection of control variates (see Equation (E.1)) and show that they satisfy the first condition in Assumption A.3.
2. More generically, we isolate the “difficult part” in our proof and provide a simple and quick algorithm that can verify the condition on a case-by-case basis for most collections of control variates; see Remark A.6 for details.

We recall that adding additional control variates makes it harder to verify Assumption 2.2, but easier to verify Assumptions 2.6 and 2.4 with good constants. For this reason, having a collection of control variates for which Assumption 2.2 is easily satisfied can lead to substantially sharper bounds for specific algorithms.

**4.2. Non-Examples.** Our main model assumption, 2.2, does not always hold. The typical problem is that some low-dimensional summary statistic is “almost sufficient.” For genuine sufficient statistics, the problem is clear:

**Example 4.3** (Sufficient Statistics). Consider a Gaussian model

$$p(\theta \mid y) \propto e^{-\theta^2} \prod_{i=1}^{n} e^{-(y_i - \theta)^2}$$

and the usual sufficient statistic $T_1(Y) = n^{-1} \sum_{i=1}^{n} y_i$. Using the notation of Assumption 2.2,

$$\mathbb{P} \left[ \| p(\cdot \mid Y^{(1)}) - p(\cdot \mid Y^{(2)}) \|_{\text{TV}} > 0 \mid \mathcal{A} \right] = 0.$$
The same problem can appear in a more subtle form: even models that exhibit large posterior fluctuations for “typical” data sets may exhibit very small fluctuations for “extremely atypical” datasets. In other words, summary statistics that do not obviously look like sufficient statistics can behave in a way that is quantitatively indistinguishable from the behaviour of sufficient statistics. Fortunately, these “bad” datasets are very rare for reasonable data generating models. In other words, the data lie in the “good” set $E$ in our Assumption 2.2 w.e.p., and the event $E$ precludes such pathological sequences of statistics. We give a somewhat cartoonish example to avoid difficult computations:

**Example 4.4 (Exponentially Unlikely Data).** Consider the light-tailed model and prior

$$p(y \mid \theta) \propto \prod_{i=1}^{n} e^{-\theta |y_i|}, \quad p_0(\theta) = e^{-\theta}$$

with $\theta \in (0, \infty)$ and $y_i \in \mathbb{R}$. Let $Y^{(1,n)} = (Y_1^{(1)}, \ldots, Y_n^{(1)})$, $Y^{(2,n)} = (Y_1^{(2)}, \ldots, Y_n^{(2)})$ be two datasets drawn from the model with “true” parameter $\theta_0 = \frac{1}{2}$. Define the summary statistic $T_n(x_1, \ldots, x_n) = \max(x_1, \ldots, x_n)$; note that this is clearly not a sufficient statistic.

Define $S_{n,k} = \sum_{i=1}^{n} |Y_i^{(k)}|, \ k \in \{1, 2\}$ and $\delta_n = e^{n^2 t(n)^{-1}}$ for some sequence $t(n) \geq e^{n^4}$. Conditional on the sequence of events $\{T_n(Y^{(k,n)}) = t(n)\}$, standard large-deviation results tell us that the event

$$\left\{ \left| \frac{S_{n,k}}{t(n)} - 1 \right| \leq \delta_n \right\}$$

holds w.e.p. On this event, we also have the event

$$\{p(\theta \mid Y^{(k,n)}) = t(n)(1 + O(\delta_n))e^{-\theta t(n)(1+O(\delta_n))}\}.$$

Directly calculating the total variation distance, we find that on this event we also have

$$\{\|p(\cdot \mid Y^{(1,n)}) - p(\cdot \mid Y^{(2,n)})\|_{TV} = e^{-\Omega(n)}\}.$$  \hfill (4.3)

Thus, we have seen that, conditional on the sequence of events $\{T_n(Y^{(k,n)}) = t(n)\}$, the sequence of events (4.3) holds w.e.p. Of course, the event $\{T_n(Y^{(k,n)}) \geq e^{n^4}\}$ has (tail) probability zero, so the introduction of the “good” set $E$ allows us to essentially discount the existence of such “bad” sequences of data in all of our proofs.

**Example 4.5 (Densely-Observed Processes).** So far, all of our data $((X_1, Y_1), (X_2, Y_2), \ldots)$ has been i.i.d. In this setting, we generally expect each datapoint to have a
substantial contribution to the posterior distribution. This can easily fail to occur for far-from-i.i.d. data. To give an informal example, consider dense observations \( \left\{ \left( \frac{i}{n}, f \left( \frac{i}{n} \right) \right) \right\} \) from a Gaussian process on \([0, 1]\). Under reasonable conditions on the prior and data-generating process, the contribution of the middle data-point \((0.5, f(0.5))\) to the posterior will often decay super-polynomially quickly.

As a consequence, we expect that subsampling MCMC algorithms, such as the recent clever work in [SQK+19], may be able to give accurate inferences based on very small subsamples in this regime.

We expect that subsampling MCMC would essentially be avoided in the situations described in these examples: a practicing statistician could compute very accurate posterior distributions by ignoring most of the the data set and using only a fixed subsample and the summary statistic \( T(Z) \).

We recall here one caveat that might be an interesting avenue of research. As pointed out in e.g. [Mon15], there are realistic situations in which computations using low-dimensional sufficient statistics are much harder than computations with the original high-dimensional data set. On the other hand, the application in [Mon15] does appear to lend itself to an efficient subsampling algorithm. However, in this application the data are not independently generated as they are in our examples, as well as most of those in the approximate MCMC literature. Thus, it is plausible to us that certain subsampling algorithms would converge extremely quickly (as they avoid our main results) while remaining practical (as direct computations with sufficient statistics are not feasible), though perhaps only for data generation processes that differ from those considered here. We are not aware of research in this direction.

5. Examples: Algorithms

In writing our main results, we deliberately avoided making detailed assumptions about how the underlying Markov chain is computed. Thus, our results apply as stated to the many algorithms in the existing subsampling MCMC literature, and no further theorems are required for specific algorithms.

In this section, we discuss some specific classes of subsampling algorithms and use them to illustrate some (non-)consequences of our results for specific popular algorithms. Although we include a few computations and theorems in this section, they are included only as illustrations. We have made no attempt to find the weakest possible conditions under which our conclusions hold and have favoured including a variety of simple proofs over optimal constants.

We note that the main difficulty in applying our results to specific algorithms is verifying Assumption 2.11 for a reasonable sequence \( \{s^{(n)}\} \). In the current
section, we use some simple algorithms to illustrate how this can be done. Detailing more complicated algorithms is beyond the scope of the current paper, but Section E in the appendix includes a generic construction and bound that we would suggest for readers interested in obtaining sharp estimates for such algorithms.

5.1. Inexact Minibatching MCMC. This paper was inspired by [KCW14] and the outpouring of related work. We begin by writing down a very simple and fairly generic subsampling algorithm that includes as special cases many subsampling algorithms in the literature, including Algorithm 1 of [KCW14], the stochastic gradient Langevin algorithm of [WT11], some but not all of the pseudomarginal-based algorithms of [QVK19], and many others.

For a finite set $S$, define $C_k(S)$ to be the uniform measure on size-$k$ subsets of $S$ and $2^S$ to be the collection of all subsets of $S$. Fix a model with parameter space $\Theta \subset \mathbb{R}^m$ and a dataset $X = (X_1, \ldots, X_n)$. The algorithm itself is written in terms of three functions $F_1 : \Theta \times [0, 1]^2 \times 2^X \mapsto [0, 1]$, $F_2 : \Theta \times [0, 1] \times 2^X \mapsto \Theta$, and $F_3 : \Theta^2 \times [0, 1] \times 2^X \mapsto \{0, 1\}$ and two parameters $k \in \{1, 2, \ldots, n\}$ and $\alpha > 0$, which will be explained below.

Our “generic” subsampling algorithm is defined by Algorithm 1, which describes a forward-mapping representation for sampling from the kernel $K(\theta, \cdot)$.

| Algorithm 1 | Generic subsampling |
|-------------|---------------------|
| 1: Sample driving randomness $U = (U_1, U_2) \sim \text{Unif}([0, 1]^2)$ and initial set $Y \sim C_k(X)$. |
| 2: while $F_1(\theta, U, Y) > \delta$ do |
| 3: Sample $Y^* \sim C_k(X\setminus Y)$ and set $Y = Y \cup Y^*$. |
| 4: end while |
| 5: Propose $\theta^* = F_2(\theta, U_1, Y)$. |
| 6: if $F_3(\theta, \theta^*, U_2, Y) = 0$ then |
| 7: Return $\theta^*$. |
| 8: else |
| 9: Return $\theta$. |
| 10: end if |

We informally relate this to the “usual” and less-abstract ways to write down MCMC algorithms:

1. Metropolis-Hastings algorithms are usually written with two sources of driving randomness; $U_1$ is the driving randomness for proposing the next state, and $U_2$ is the driving randomness for accepting/rejecting this proposal.
(2) The function $F_1$ is a measurement of how well $Y$ approximates the entire dataset $X$, and $\delta$ is a threshold for how good this approximation must be.

(3) The function $F_2$ is the forward-mapping representation for the proposal kernel.

(4) The function $F_3$ approximates the usual accept/reject rule with Metropolis-Hastings acceptance probability $\alpha(\theta, \theta^*)$.

We would like to study when our main results give an interesting conclusion about this algorithm - in particular, for which sequences $m(n)$, $s(n)$ Algorithm 1 satisfies Assumption 2.10. This is quite a broad question, so we consider the important but simple case where all datapoints influence the algorithm and it is rare to use very large subsamples:

**Assumptions 5.1.** Assume that the subsampling algorithm satisfies

1. The output of the algorithm depends on every component of the sampled $Y$ for every value of $U$.
2. For all $n$, the distribution of the number of steps $N$ in the “while” loops has CDF $F^{(N)}$ that satisfies

   $$1 - F^{(N)}(x) \leq e^{-\lambda_2^{-1}(x-\lambda_1)}$$

   for some constants $0 < \lambda_1, \lambda_2 < \infty$. In other words, $N$ is stochastically dominated by a constant $\lambda_1$ plus an exponential random variable with mean $\lambda_2$. Define $\lambda = \lambda_1 + \lambda_2$.  

As Algorithm 1 is written above, it is straightforward to check that we must in fact choose $s \equiv 1$ under Assumption 5.1; that is, we must use all of the data at every iteration. Fortunately, this problem occurs only because Algorithm 1 is a rather unsuitable representation of the kernel. This can be remedied by choosing another kernel that represents the same Markov chain but gives better constants:

**Proposition 5.2.** Let Assumptions 5.1 hold and fix constants $0 < \epsilon < 1$, $m(n) \equiv m \in \mathbb{N}$. Then there exists a representation of the Markov chain defined in Algorithm 1 for which Assumption 2.10 holds with

$$s(n) = C n \log(n),$$

where $C = C(\epsilon, \lambda, k, m) \equiv \frac{1 - \epsilon}{\lambda k m}$.  

**Proof.** See Appendix D for a proof, including an explicit construction of the forward-mapping representation.  

Note that this assumption allows for a deterministic sample size.
Proposition 5.2 is important for two reasons. First, it implies a lower bound on the computational cost that is linear in \( n \), with no logarithmic factors. Second, it illustrates the fact that the natural representation of an algorithm may not give the best estimates. Although we study Assumption 2.10 in this comment, essentially the same construction can be used to give the same bounds using its alternative Assumption 2.13.

5.2. **Exact Minibatching MCMC.** To our knowledge, the first exact-approximate subsampling algorithm that applied in some generality was the FlyMC algorithm of [MA14]. Theorem 3 applies quite directly to this algorithm, showing that the spectral gap of this algorithm must be rather small for problems such as logistic regression. We give a few additional comments on how our results relate to this algorithm. Throughout, we mimic the notation of [MA14], but to save space we don’t restate the full algorithm.

5.2.1. **Lower and Upper bound functions.** The algorithm of [MA14] involves the computation of lower and upper bound functions \( L_n, B_n \) that satisfy \( L_n(\theta) \leq p(\theta | Z) \leq B_n(\theta) \). When applying Theorem 3, we view \( L_n \) and \( B_n \) as being further pre-computed control variates. This presents no difficulty for our framework.

5.2.2. **Convergence of Full and Reduced Markov Chains.** Theorem 3 applies to the mixing of the full FlyMC Markov chain. However, FlyMC is a data-augmentation algorithm; the associated Markov chain may be written in the form \( \{ (\theta_t, \omega_t) \}_{t \in \mathbb{N}} \), where \( \mathcal{L}(\theta_t) \) converges to the posterior distribution \( p(\theta | z) \) and \( \omega_t \in \{0, 1\}^n \) is a collection of auxiliary variables that is generally ignored after the computation is complete.

For statistical applications, we are only interested in the mixing of the sequence \( \{ \theta_t \}_{t \in \mathbb{N}} \). It is natural to ask: could FlyMC as a whole mix slowly while \( \{ \theta_t \}_{t \in \mathbb{N}} \) mixes quickly? If so, this would make our lower bound on the mixing rate much less relevant and allow for the possibility of an efficient FlyMC algorithm. Unfortunately, the answer is often **no** in the case of FlyMC.

This is easiest to see in the special case that the parameter \( \text{ResampleFraction} = 1 \) in their Algorithm 1, so that the entire subsample is refreshed at each iteration. In this case, the first coordinate \( \{ \theta_t \}_{t \in \mathbb{N}} \) is in fact a Markov chain. By Theorem 3.3 of [LWK94] the spectral gap of this chain is equal to the spectral gap of the joint chain \( \{ (\theta_t, \omega_t) \}_{t \in \mathbb{N}} \), and so it cannot mix more quickly. The same argument gives the same conclusion for the improved Algorithm 2 of [MA14].
5.2.3. Typical covering times. In Theorem 1, the bound on the relaxation time depends on the (random) time $\tau_z$ required to see almost all of the dataset. This number is often substantially larger than the number of datapoints $n$ divided by the mean number of datapoints seen per step of the Markov chain.

We give a simple illustration in the context of [MA14]. Assume that the lower and upper bound functions $L_n, B_n$ used in Algorithm 1 of [MA14] satisfy

$$\epsilon < \frac{L_n(\theta)}{B_n(\theta)} < 1 - \epsilon \quad (5.2)$$

for some $0 < \epsilon < \frac{1}{4}$ and all $\theta \in \Theta$. Then, by the well-known coupon-collector calculation,\(^7\)

$$\frac{1}{2} \log(n) \leq \tau_z \leq \frac{2}{\epsilon} \log(n) \quad (5.3)$$

holds w.e.p., while the average number of datapoints used per transition is on the order of $cn$ for some $\epsilon \leq c \leq 1 - \epsilon$. Thus, returning to Theorem 1, we see that in fact the ratio of relaxation time to average number of datapoints per step scales linearly in $n$. This is slightly better than the naive lower bound of $\Omega(\frac{n}{\log(n)})$ on the scaling rate.

The uniform bound (5.2) is quite strong, and will not hold in all applications. Improving on this is far beyond the scope of this paper, but we note that well-known variants of the coupon collector problem tell us that the conclusion (5.3) holds under much weaker conditions than (5.2). In particular, having (5.2) for a positive fraction of the values of $\theta$ is enough, and this covers many more cases of practical interest.

5.3. Informed Subsamplers. In Algorithm 1, the subsamples used at each step are chosen uniformly and independently. In many approaches to subsampling, this does not hold. To give two extreme examples, [HCB16] simply chooses a subset of the data and ignores the rest, while [MFA19] allows any subsample to be chosen at any step but “upweights” certain datapoints based on some pre-computed measure of informativeness.

Because these algorithms can’t easily be put into a form similar to Algorithm 1, the discussion in Section 5.1 doesn’t apply directly. The place where this difference is most significant is in the estimation of typical covering times. We consider a simplified version of [MFA19], obtained by modifying a single line of Algorithm 1: rather than sampling $Y \sim C_k(S)$ in that algorithm, we sample

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\(^7\)See [Erd61].
a subset $Y$ of $S$ of size $k$ according to weights of the form

$$\mathbb{P}[Y = y] \propto \prod_{i=1}^{k} w(y_i; \theta)$$ (5.4)

for some pre-computed weights $w$.

Since this algorithm does not have the same form as Algorithm 1, we can’t directly apply the theory in Appendix D and so we don’t have a similar proof of Proposition 5.2. We see no way to write a completely general version of this algorithm for which Assumptions 2.2 and 2.10 hold for large $s(n)$.

However, under a small strengthening of our assumptions, we can use Assumptions 2.13 and 2.12 in place of Assumptions 2.2 and 2.10, obtaining large values of $s(n)$. Our first assumptions are:

**Assumptions 5.3.** Fix parameters as in Assumption 2.2, and let $p_n$ be the probability that Inequality (2.8) fails to hold under this assumption.

Fix also $1 \leq A < \infty$ and weights $w$ as in Equation (5.4) that satisfy

$$A^{-1} \leq \sup_{\theta \in E} \sup_y w(y; \theta) \leq A.$$ 

We assume that

$$\sum_n p_n A^{-8mA^4 \log(n)} < \infty.$$ (5.5)

Inequality (5.5) is simply a quantitatively-stronger version of an event happening w.e.p., and so Assumption 5.3 is essentially a quantitatively-stronger version of Assumption 2.2. This condition is not implied by Assumption 2.2, but our existing arguments for Assumption 2.2 (as summarized in Section 4) can be modified to prove Inequality (5.5).

This assumption leads to:

**Proposition 5.4.** Consider a Markov chain of the form 1, but with all draws from $C_k$ replaced by draws from the weighted measures defined in Equation (5.4). Let Assumptions 5.1 and 5.3 hold. Also assume that $F_1 \equiv 1$, so that only a single subsample is used at every step. Finally, fix $m(n) \equiv m \in \mathbb{N}$. Then Assumptions 2.13 and 2.12 hold with

$$s(n) = Cn \log(n),$$ (5.6)

for some constant $C = C(\lambda, k, m)$ independent of $n$.

**Proof.** See Appendix D.
6. Discussion

We have given various “no-free-lunch” theorems for subsampling MCMC, showing that subsampling MCMC can’t give “large” improvements under some conditions. We summarize our main message: for reversible MCMC algorithms and statistical models such as GLM, subsampling and approximate MCMC don’t “work” - you either don’t get much speedup (compared to the associated exact chain) or have estimates that aren’t much better (compared to doing inference based on just your control variates).

To us this feels like an argument for focusing primarily on control variates over attempts to do clever subsampling schemes, when our results apply. In this section, we discuss several situations in which our results don’t apply. We also lay out the most important questions that are left open by this paper.

6.1. Free Lunches for Highly Nonreversible Chains. Our main result for reversible chains, Theorem 3, is quite easy to interpret: it says that, if you choose a family of subsampling Markov chains in advance, most of the associated Monte Carlo averages will have large asymptotic variance. Our result for nonreversible chains is much harder to interpret, and we consider this the most important open problem left by this paper.

The basic problem is that, for reversible chains, the following are all characterized by the spectral gap:

1. The total variation mixing time from a “warm start” (see Theorem 2).
2. The medium-time error of an estimator for the “worst” test function (see e.g. Proposition 3.8 of [Paul15], though other results along these lines exist).
3. The asymptotic variance of an estimator for the “worst” test function (see e.g. [Jon04] and the references therein).

Since the three different notions of mixing are all characterized by a single quantity, we can get a bound on the spectral gap by taking advantage of the first property and know that it is relevant to the accuracy of our Monte Carlo estimators by using the third property.

In the nonreversible case, these three notions of mixing may be very different. We chose to focus on one of the best bounds on the Monte Carlo error over medium time scales that we know of, as given by Proposition 3.4 of [Paul15] in terms of the pseudospectral gap. Qualitatively similar results are easy to obtain for various other summary measures of a nonreversible Markov chain’s performance, using essentially the same methods. See e.g. [KM12], [KM05], [KM03] for relationships between the spectral theory and long-time
asymptotics of nonreversible Markov chains, and [MT06], [Cho17] for some discussion of the short- and medium-time mixing properties.

Our understanding is that the pseudospectral gap is a good proxy for the convergence rate of Monte Carlo ergodic averages of many simple “quickly-mixing” nonreversible chains, and we conjecture that this is also true for some proposed nonreversible subsampling MCMC chains. However, we emphasize that we do not know if this is true, and there is some strong evidence against this heuristic. For example, there are many examples in the literature of nonreversible chains for which these two quantities are very different. Even worse for our assertion, some of these can be cast as subsampling chains! As an extreme example, the herded Gibbs sampler of [CBDF+16] is used to sample from a Markov random field on a graph. If we imagine a sequence of graphs for which the number of vertices goes to infinity while the maximum degree remains bounded, these Gibbs samplers use only $O(1)$ data points per step and Theorem 4 applies. However, the bound in that theorem is misleading: the herded Gibbs sampler is deterministic, and has no (pseudo)-spectral gap at all, but the associated ergodic averages converge extremely quickly even for large data sets.

The main open problem left by our work can be summarized as: can the phenomenon that occurs for [CBDF+16], where the (pseudo)-spectral gap is not even close to determining the convergence rate for ergodic average, occur for more general target measures and subsampling algorithms?

6.1.1. Relationship to Existing Heuristics. We note that various heuristic arguments have been put forward to explain the good performance of subsampling-based MCMC algorithms. In this section, we recall these heuristics and give a quick illustration of why they don’t appear to answer our open question. The heuristic we present below is based on our understanding of the informal argument in Section 5 of [BFR16], where it is applied to their zig-zag process. We suggest interested readers go through their more detailed discussion, as our present version is necessarily shorter and simpler; we also note that very similar arguments also apply to e.g. [WT11, KCW14] with appropriate control variates and target distributions.

We continue by considering the special case studied in Theorem 1: our data is drawn from some “nice” logistic regression model, and we wish to run a subsampling MCMC algorithm targeting a “very good” approximation of the true posterior distribution. We also precompute the MLE for this model, as well as the Hessian at the MLE, and allow the subsampling MCMC algorithm to use these precomputed values as control variables. The heuristic convergence argument has the following basic form:
(1) After appropriate rescaling, the target distribution and the transition kernel of the MCMC algorithm converge to a standard Gaussian and some limiting kernel as the amount of data goes to infinity.

(2) The limiting kernel is geometrically ergodic, with stationary measure equal to the standard Gaussian.

(3) Since the limiting kernel doesn’t include any terms related to the size of the dataset $n$, its convergence rate is independent of $n$.

(4) Since the individual kernels converge to the limiting kernel, they should inherit its mixing properties; therefore, the convergence rates of the individual kernels should be bounded uniformly in $n$.

This argument is informal, and the authors of the above papers have not claimed otherwise. The main difficulty is clearly in going from step (3) to step (4) - its correctness depends on exactly how the various types of convergence are measured. Although this heuristic doesn’t immediately yield a theorem, it did seem fairly convincing to us at first glance (and even at third glance).

However, we have already seen that the computational cost of subsampling MCMC scales like at least $\Omega\left(\frac{n}{\log(n)}\right)$ for a broad class of reversible MCMC chains, and that the pseudospectral gap also shrinks at least this quickly for non-reversible chains. In other words: for a variety of algorithms including both [BFR16] and [WT11, KCW14], the informal argument does not give the “right” answer for some measures of the rate of convergence (in particular, the pseudospectral and spectral gaps respectively).

This leads us to the following very concrete open problem. Our favourite version of this informal argument appears in Section 5 of [BFR16], where it is written very clearly (and where there are several clear caveats). The results of our paper tell us that the pseudospectral gap doesn’t converge as this informal argument would suggest. However, we are not able to draw any conclusions at all about the convergence rate of ergodic averages. Our main question is:

**What is the convergence rate of ergodic averages for the process described in [BFR16] applied to GLMs, for example?**

6.1.2. Further Subsamplers. Although we have focused on the zig-zag process, we note that there has been quite a lot of work recently on the development of other subsamplers that are not reversible Markov chains. We give brief comments on how our results apply or fail to apply.

Several recent papers, including [BFR16] and [BCVD18], propose continuous-time Markov processes that occasionally “change directions” at random times that are more likely to occur in low-density regions of the target distribution. While our results do not apply to the original continuous-time process, they do give bounds on the pseudospectral gap for the discrete-time “skeleton” chain...
that records the location and time of each direction change. As a result, the basic conclusions apply.

The ScaLE algorithm of [PFJR16] is a recent and very promising approach to subsampling Monte Carlo. This algorithm is based on the convergence of a Markov process with killing to its quasistationary distribution, rather than the convergence of a Markov process without killing to its stationary distribution. As such, Theorems 3 and 4 do not apply directly.

We outline the technical problem. The main ingredient of our simple proofs is the “warm start” bound of Theorem 2. We are not aware of any analogous bound for the convergence of Markov processes with killing to their quasistationary distributions (though see e.g. [VD91, DM14] for analogous results for discrete Markov chains). Such a bound would be implied by any sensible estimate of the constant $C$ appearing in Theorem 2 of [WKSR17].

6.2. Free Lunches for Very Expensive Posteriors. Like the existing literature, we have focused on posterior distributions with the product form

$$p(z \mid \theta) = p(\theta) \prod_{i=1}^{n} p(z_i \mid \theta).$$

For such distributions, the per-step cost of a subsampled chain scales like the number $m$ of datapoints used, while our results say (very roughly) that the relaxation time scales like $\frac{n}{m}$ at best. Taking these facts together, this implies that the computational cost per effectively-independent sample from any exact subsampling step must be roughly $\Omega(n)$, regardless of the value of $m$.

However, if we consider more computationally expensive posterior distributions with costs scaling like $m^c$ for some $c > 1$, this conclusion disappears: the same heuristic allows for a cost reduction from $\Omega(n^c)$ to $O(n)$ in the case that $m = O(1)$. We suspect this is a fruitful avenue for future research, and note that the types of problems studied in [Mon15] often fall into this category.

6.3. Cheaper Lunches for Systematic Data Scans. In principle, Theorem 1 allows speedups by a factor of $\log(n)$. In Sections 5.2 and 5.3, we saw that even this logarithmic speedup is impossible when only a small random subsample of data is used at each step.

This problem is reminiscent of the problem of choosing the scan order for Gibbs samplers. By essentially the same “coupon-collector” calculation referenced in Sections 5.2 and 5.3, the mixing time of any random-scan Gibbs sampler targeting a density supported on $\mathbb{R}^d$ must be at least $\frac{1}{2}d \log(d)$. It
is well-known that systematically scanning coordinates in order can sometimes give a Markov chain with mixing time that is $\Theta(d)$. Unfortunately, this speedup is somewhat subtle, and in some cases systematic scans can be slower than random scans (see further discussion in [RR15]). We suspect a similar phenomenon for subsampling MCMC: systematic scans might be able to give a speedup of roughly $\log(n)$ for some examples, but we expect this speedup to be delicate and quite problem-specific.

6.4. **Free Lunches for Data Augmentation.** Many approximate MCMC algorithms are defined on augmented state spaces. Our results imply that the full MCMC algorithms cannot mix too quickly, but in principle it is possible that all statistically-relevant functions of the chain do mix quickly.

We are not aware of any realistic situations in which this occurs, and in Section 5.2, we used [LWK94] to show that this can’t occur for a specific algorithm. In general, however, this question appears to be open.

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Appendix A. Models with Large Fluctuations and Warm Starts

We begin by giving some generic conditions under which our “warm start” and “large fluctuation” assumptions hold (see Sections A.1 and A.2 respectively). We then apply these to prove Theorem 6, our main result on logistic regression, in Section A.3. Finally, Section E gives some suggestions on constructing “additional” control variates.

We note that the main obstacle in extending Theorem 6 to other models and control variates occurs in Section A.2. See that section for an overview of the main difficulties, including an algorithm for using a computer to verify the main conditions for specific examples.

A.1. Warm Starts. We introduce sufficient conditions for warm starts that apply to all GLMs considered in the current paper, and many other models. Define $B_r(x) = \{y : \|x - y\| \leq r\}$ to be the usual ball of radius $r$ around $x$.

**Lemma A.1.** Let $\{\nu_n\}_{n \in \mathbb{N}}$ be a sequence of measures on $\mathbb{R}^d$ with densities $\{p_n\}_{n \in \mathbb{N}}$. Assume there exist constants $\delta, c, N_0$ so that

1. For $n > N_0$, $p_n$ has a unique maximizer $\hat{\theta}_n$.
2. For $n > N_0$, $\nu_n(B_1(\hat{\theta}_n)) > 0.5$.
3. For all $n > N_0$,
   \[ \sup_{\|\theta - \hat{\theta}_n\| \leq \delta} \sup_{\|v\| = 1} \frac{|\nabla_v p_n(\theta)|}{p_n(\theta)} \leq n^c. \] (A.1)

Then the sequence of measures $\text{Unif}(B_{n^{-c}}(\hat{\theta}_n))$, with densities $\lambda_n$, satisfies

\[ \frac{\lambda_n(\theta)}{p_n(\theta)} \leq Cn^{cd} \] (A.2)

for some constant $C$ that does not depend on $n, c$ or $d$.

**Proof.** Note that, for any $0 \leq r < \delta$ and $\theta \in B_r(\hat{\theta}_n)$, we have by Inequality (A.1) and Grönwall’s inequality

\[ p_n(\theta) \geq e^{-rnc} p_n(\hat{\theta}_n). \]

In particular, choosing $r(n) = n^{-c}$,

\[ p_n(\theta) \geq e^{-1} p_n(\hat{\theta}_n), \quad \forall \theta \in B_r(\hat{\theta}_n) \] (A.3)

for all $n > N_0 \lor \delta^{-1/c}$. Also for $n > N_0$, we have by assumption that $\nu_n(B_1(\hat{\theta}_n)) > 0.5$. Then it follows that

\[ 0.5 < \nu_n(B_1(\hat{\theta}_n)) < p_n(\hat{\theta}_n) \text{Vol}(B_1(\hat{\theta}_n)) \]
\[ p_n(\hat{\theta}_n) > 0.5 \frac{\Gamma(d/2 + 1)}{\pi^{d/2}} \]

On the other hand
\[
\lambda_n(\theta) = \frac{1}{\text{Vol}(B_{r(n)}(\hat{\theta}_n))} = r(n)^{-d} \frac{\Gamma(d/2 + 1)}{\pi^{d/2}}
\]

Giving
\[
\frac{\lambda_n(\theta)}{p_n(\theta)} < \frac{r(n)^{-d}}{e^{-0.5}r(n)^{-d}} = 2en^{cd}.
\]

\[\Box\]

Note that posterior distributions themselves will generally not satisfy the conditions of this lemma. However, if \( q_n \) is a posterior distribution, we expect that \( p_n(\theta) \equiv q_n(B_n(\theta - a_n)) \) will satisfy the conditions for appropriate choice of \( a_n \in \mathbb{R}^d \) and \( B_n \) a \( d \times d \) matrix with operator norm \( \|B_n\| = n^O(1) \), which is sufficient to recover the required warm start condition by applying the chain rule. In the context of this paper, we choose the same \( a_n, B_n \) as appears in the Bernstein-von Mises theorem (see e.g. [LCY12]8).

Although it is beyond the scope of this paper to survey this literature, there is a large literature on similar “warm start” conditions, and much stronger results are possible. For example, Section 9 of [Vem05] gives a construction of a distribution that satisfies a far stricter “warm start” condition for a very broad class of distributions.

In the special case of logistic regression, we recall that the posterior distribution for logistic regression with suitable prior is log-concave. When the posterior also converges (upon rescaling) to a standard Gaussian, very strong results on log-concavity, such as Proposition 2 of [CS10], imply that a bound of the form Inequality (A.2) holds with the right-hand side replaced by some absolute constant that does not depend on \( n \) or \( d \).

### A.2. General Sufficient Condition for Large Fluctuations

In this section, we give some notation and generic sufficient conditions for Assumption 2.2 to hold. Throughout the section, fix notation as in that assumption, and view \( E = \{E^{(n)}\}, m = \{m^{(n)}\} \) as belonging to a sequence indexed by \( n \in \mathbb{N} \); we view the constants \( c_1, C_1 \) as fixed for all \( n \). We will primarily be concerned

\[\footnote{A small warning to the reader uninitiated in asymptotics of the MLE: as discussed in [LCY12], actually verifying convergence to a Gaussian with nonrandom normalizing sequences is surprisingly time-consuming. However, our theorem above requires only tightness of the posterior distributions, and so merely having a bounded sequence of normalizing constants is enough.}
with regression-like models, so we assume that $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$, where $\mathcal{X} = \mathbb{R}^d$ for some $d \in \mathbb{N}$.

Rather than giving a minimal-length proof of our application in the main text, we give a collection of conditions that will be more useful to readers who wish to establish large fluctuation conditions for their own models. We give these conditions in two parts. In Section A.2.1, we give some generic “geometric” conditions stated in terms of objects such as manifolds, tangent spaces and so on associated with the model; see Assumption A.3. In Section A.2.2, we specialize to the case of GLMs and give simple conditions on the model that imply these geometric conditions; see Assumption A.5. Between these two sections, we hope to illustrate that the large fluctuation condition is both (i) fairly generic, even for models that don’t look much like GLMs and (ii) often straightforward to verify for popular models. We note that the conditions in these sections are still far from optimal - for example, the conditions are based on taking various derivatives, so they don’t apply to discrete covariate data.

We note that the main technical difficulty throughout essentially all of this section comes from the fact that we are conditioning on the values of the test statistics $T_1, \ldots, T_k$. This will generally restrict our allowed data to some implicitly-defined submanifold, and we must confirm that this submanifold is not too badly-behaved (primarily that it is well-approximated by its tangent planes on a sufficiently large scale). In the end, this boils down to verifying that a certain random matrix with highly dependant entries is not very close to singular; this seems to often be true, but such random matrices are not easy to analyze using currently-available tools. While this presents a major mathematical difficulty towards obtaining a general theory, it is fortunately simple to check on a case-by-case basis. Remark A.6 immediately follows the condition that is difficult to verify, explains the difficulty, and gives a straightforward (and very fast) algorithm for verifying it for any specific model.

A.2.1. Geometric Conditions for Large Fluctuations. Roughly speaking, we expect a large fluctuation condition to hold if the following hold at “most” points:

(1) It is possible to perturb the data by some small amount, while still holding the test statistics constant (see the first part of A.3).

(2) Most small perturbations to the data give similar-size perturbations to the posterior density at most points (see the rest of A.3).

This section’s main result, Lemma A.4, is a precise statement of this heuristic. For any fixed collection of test statistics $T_1, \ldots, T_k$, covariate data $X =$
(x_1, \ldots, x_n) \in \mathcal{X}^n, \text{ response data } Y \in \mathcal{Y}^n \text{ and integer } 1 \leq m \leq n, \text{ define}
\mathcal{G} = \mathcal{G}(X) = \{ G = (g_1, \ldots, g_n) \in \mathcal{X}^n : T_i(G, Y) = T_i(X, Y) \forall i \leq k, g_{1:m} = x_{1:m} \}

\text{to be the collection of extensions of } x_{1:m} \text{ that keep the existing statistics } T_1, \ldots, T_k \text{ fixed. In other words, this is the set of all sequences of length } n \text{ having both the same statistics and the same first } m \text{ elements. We note that we are suppressing the response data } Y \text{ in this notation. This is largely for convenience: our proof results are based on taking derivatives of various objects, and in our prototypical example } Y \text{ takes on discrete values. We resolve this tension by viewing } Y \text{ as fixed (rather than random) throughout the following calculations. We denote by } \gamma_{n,Y} \text{ the conditional distribution of } X \text{ given these observed response variables. Finally, we note that } \mathcal{G}(X) \text{ is determined by any of its elements: for all } X \text{ and all } X' \in \mathcal{G}(X), \text{ we have } \mathcal{G}(X) = \mathcal{G}(X').

We now make an assumption about the “inner curvature” of } \mathcal{G}. \text{ Before giving a formal definition of inner curvature, we give a very special case that is easy to understand: when } \mathcal{G} \text{ can be written in the form } \mathcal{G} = \{(x, f(x)) : x \in \mathbb{R}\} \text{ for some } f : \mathbb{R} \mapsto \mathbb{R}, \text{ the inner curvature of } \mathcal{G} \text{ is just } \sup_x |f''(x)|^{-1/2}.

We say that an embedded manifold } M \text{ in Euclidean space has } \text{strong inner curvature} \text{ at least } c > 0 \text{ if, for all } x \in M \text{ and all balls } B \text{ tangent to } M \text{ at } x \text{ with radius } c, \text{ we have } M \cap B = \{x\}. \text{ We need to slightly relax this condition to allow for the possibility that } M \text{ has self-intersections or otherwise “loops back” on itself:}

\textbf{Definition A.2.} \text{ We say that a closed subset } M \text{ of Euclidean space has } \text{inner curvature} \text{ at least } c > 0 \text{ if there exists an open cover of } M \text{ by embedded manifolds } \{U_\alpha\}_{\alpha \in \mathbb{N}}, \text{ and furthermore this open cover satisfies:}

(1) \text{ For every ball } B \text{ of radius } c, \text{ there exists } \alpha \in \mathbb{N} \text{ so that } B \cap M \subset U_\alpha.

(2) \text{ For every } \alpha, U_\alpha \text{ has strong inner curvature at least } c.

This condition may look intimidating at first, but our manifold of interest } \mathcal{G}(X) \text{ is rather special: it is exactly the set on which a collection of equations defined by } T_1, \ldots, T_k \text{ is constant. In the end, this means that it is possible to check that } \mathcal{G}(X) \text{ has inner curvature at least } c > 0 \text{ by doing some fairly explicit computations involving derivatives of } T_1, \ldots, T_k. \text{ Roughly speaking, we can use the implicit function theorem to find a local parameterization of } \mathcal{G}(X) \text{ in terms of these functions, and then verify the inner curvature condition by finding a lower bound on the smallest singular value of the Jacobian of this parameterization. The details of this strategy are carried out in Lemma A.9.}

Informally, having inner curvature } c > 0 \text{ means that we can travel the manifold } M \text{ along the direction of tangent spaces in the “obvious” way up to
distances of about \( c \) without encountering problems. We now formalize what we mean by the “obvious” way. For \( x \in \mathcal{M} \), define \( \alpha(x) = \min\{ \beta \in \mathbb{N} : B_c(x) \cap \mathcal{M} \subset U_\beta(x) \} \), where we recall \( B_c(x) \) is the ball of radius \( c \) around \( x \) and the minimum appears in this definition solely to provide some measurable function that chooses a single element of the cover. For \( x \in \mathcal{M} \) and unit vector \( v \), define the function \( \psi_{x,v} : \mathbb{R} \mapsto U_{\alpha(x)} \) by

\[
\phi_{x,v}(s) = \arg\min_{x' \in U_{\alpha(x)}} \| x + sv - x' \|. \tag{A.5}
\]

This function determines short paths along \( \mathcal{M} \) that start by travelling in direction \( v \) from point \( x \). When \( \mathcal{M} \) has inner curvature \( n^{-c} \), it follows that for any \( s < n^{-c} \) and \( v \in T_x \mathcal{M} \), the tangent space of \( \mathcal{M} \) at \( x \), we have

\[
\phi_{x,v}(s) = x + s'v'
\]

for some \( s', v' \) satisfying \( |s - s'|, \frac{\|v-v'\|}{s} = O(n^c s^2) \).

Having made an assumption that it is possible to travel along \( \mathcal{G} \) in a fairly smooth way, we next make assumptions about how small changes along \( \mathcal{G} \) result in changes to the posterior. For \( m < i \leq n \), \( 1 \leq j \leq d \), \( 1 \leq \ell \leq k \) and \( X = (x_1, \ldots, x_n) \in \mathcal{X}^n \) with \( x_i = (x_{i1}, \ldots, x_{id}) \), define

\[
\dot{T}_{i,j}^{(\ell)}(X) = \frac{\partial}{\partial x_{ij}} T_{\ell}(X,Y).
\]

For \( \theta \in \Theta \), also define

\[
D_{i,j}(\theta, X) = \frac{\partial}{\partial x_{ij}} \log \{ p(\theta \mid (X,Y)) \} = \frac{1}{p(\theta \mid X,Y)} \frac{\partial}{\partial x_{ij}} p(\theta \mid (X,Y))
\]

and

\[
D_{\max}(\theta, X) = \max_{i,i',j,j'} \frac{1}{p(\theta \mid (X,Y))} \left| \frac{\partial^2}{\partial x_{ij} \partial x_{i'j'}} p(\theta \mid (X,Y)) \right|.
\]

With the same indices, define

\[
W_\ell = W_\ell(X) \equiv \left\{ v = (0, 0, \ldots, 0, v_{m+1}, \ldots, v_n) \in (\mathbb{R}^d)^n : \sum_{i=m+1}^n \sum_{j=1}^d |v_{ij}|^2 = 1, \sum_{i=m+1}^n \sum_{j=1}^d v_{ij} \dot{T}_{i,j}^{(\ell)} = 0 \right\}
\]

to be the collection of (normalized) directions that don’t influence \( T_{\ell} \) and keep the first \( m \) data points fixed, and let

\[
W = W(X) \equiv \bigcap_{\ell=1}^k W_\ell(X).
\]
Note that, by dimension-counting, we must have $\dim(\text{span}(W)) \geq d(n - m - k)$. Thus, as long as $m \leq n - k - 1$, $W$ is non-empty. We also note that, for $X' \in G$, $W(X')$ generates the tangent space of $G$ at $X'$.\(^9\)

Finally, for any set $S \subset \mathbb{R}^\ell$ and any $A > 0$, define
\[
S_A = \{ x \in \mathbb{R}^\ell : \inf_{s \in S} \| s - x \| \leq A \}
\]
to be the $A$-thickening of $S$. With this notation, we state the following simpler-to-verify sufficient conditions for Assumption 2.2:

**Assumption A.3 (Good Points).** Fix a collection
\[
\mathfrak{A} = \{ a_1, a_2, a_3, a_4, A_1, A_2, A_3, A_4, c \}
\]
of finite, positive constants satisfying $A_1, A_2, A_3, A_4 > 1$, $a_1, a_2, a_3, a_4, c \in (0, \infty)$, $x \in E$, and $v \in W$. With notation as above, say that $(x, v)$ is $\mathfrak{A}$-good if

1. **$G$ is often locally well-approximated by $W$:** $G(x)$ has inner curvature at least $n^{-c}$.
2. **Posterior Sensitivity:**
   - There exists $B_1 \subset \Theta$ so that
     \[
     \sup_{\theta \in B_1} \sup_{X : |X - x| \leq A_1^{-1} n^{-a_1}} D_{\text{max}}(\theta, X) \leq A_1 n^{a_1} \quad (A.7)
     \]
     \[
     \inf_{X : |X - x| \leq A_1^{-1} n^{-a_1}} p(B_1 | X, Y) \geq 1 - A_2 n^{-a_2}.
     \]
   - For $X$ satisfying $|X - x| \leq A_1^{-1} n^{-a_1}$, define the set of points that are not highly sensitive to perturbations:
     \[
     B_1(v, X) = \left\{ \theta \in B_1 : \left| \sum_{i,j} v_{i,j} D_{i,j}(\theta, X) \right| \in (A_3^{-1} n^{-a_3}, A_3 n^{a_3}) \right\}. \quad (A.8)
     \]
   - This set is large in the following sense:
     \[
     \lambda(B_1^c(v, X)) \leq A_4 n^{-a_4}. \quad (A.9)
     \]

\(^9\)This is a small imprecision, as we allow $G$ to have self-intersections. We deal with this rigorously by only ever using the tangent space associated with a particular element of the covering in Assumption A.2. Since the target audience of this paper may not have a lot of familiarity with differential geometry, we will continue to slightly abuse notation by e.g. talking about “the tangent space of $G$ at $y$” as a shorthand for “the tangent space of the element $U_{\alpha(y)}$ of the cover of $G$ around the point $y$” when this does not cause mathematical confusion.
(3) **Non-super-concentration of Posterior:** For any subset $S \subset \mathcal{B}_1$ with $\lambda(S) \leq A_4n^{-a_4} + A_2n^{-a_2}$, we have

$$\sup_{X : |X - x| \leq A_1^{-1}n^{-a_1}} \int_{\theta \in S} p(d\theta|x) < \frac{1}{2}.$$  \hspace{1cm} (A.10)

We give quick explanations of the purpose behind these assumptions:

(1) When $\mathcal{G}$ has positive inner curvature, it is well-approximated by its tangent space.

(2) Inequality (A.7) guarantees that the derivative $D_{i,j}$ doesn’t change too quickly near $x$. Inequality (A.8) guarantees that, by moving the data $X$ a small distance $\epsilon$ in some direction $v \in W$, we can change $p(\theta|X,Y)$ by at least $\epsilon \Delta(\theta)$ outside of a small “bad” set $\mathcal{B}_1^c(v,x)$. Furthermore, the constant $\Delta(\theta)$ is at least polynomially small and at most polynomially large in $n$.

(3) This guarantees that the small “bad” set $\mathcal{B}_1^c(v,X)$ allowed by the previous assumption is not close to covering the entire posterior mass.

More briefly, these tell us that $\mathcal{G}(X)$ looks “locally linear” and that $p(\theta|X,Y)$ responds in a “locally linear” way to small changes in $X$, at least much of the time. We now check that Assumption A.3 implies Assumption 2.2:

**Lemma A.4.** Fix $\gamma$ satisfying the first part of Assumption 4.1 and $Y$ so that $\gamma_{n,Y}$ satisfies the second part of Assumption 4.1, and also $E$, $m$ and a collection of constants $\mathfrak{A}$. Assume that a random pair $X \sim \gamma_{n,Y}$ and $v \sim \text{Unif}\{\{w \in W : \|w\| = 1\}\}$ is $\mathfrak{A}$-good in the sense of Assumption A.3 w.e.p. Then $p$ exhibits large fluctuations with the same choice of $\gamma$, $E$, $m$.

**Proof.** Throughout this proof, we view $Y$ as fixed; all calculations are done conditional on $Y$ when relevant. Next, note that we need only pay attention to points $x_1, \ldots, x_n$ in the support of $\gamma$; since this is contained in a fixed compact set by Assumption 4.1, we can assume without loss of generality that $\sup_{x \in E} \|x\|_{\infty}$ is uniformly bounded even as $n$ goes to infinity.

Fix some pair $(x,v)$ that are good in the sense of Assumption A.3. By the first part of the assumption, the tangent plane $W(x)$ to $\mathcal{G}$ shifts very little over neighbourhoods of size $o(n^{-c})$.\hspace{1cm} \text{10} Let $R = R(n) = \frac{1}{4} \min(n^{-2c}, \frac{A_3(A_1+A_3)}{A_1}n^{-a_1-a_3})$.

Fix $v \in W(x)$ and $0 \leq s \leq R(n)$. Thus, for $\theta \in \mathcal{B}_1 \cap \mathcal{B}_1(v,x)$ and all $0 \leq s < R(n)$, we have by Inequalities (A.8) and (A.7)

$$\left(A_3^{-1}n^{-a_3} - sA_1n^{a_1}\right)p(\theta|x) \leq \left|\frac{d}{dt}p(\theta \mid x + tv)\right|(0) \leq (A_3n^{a_3} + sA_1n^{a_1})p(\theta|x);$$

\hspace{1cm} \text{10To make this precise we must also avoid possible self-intersections; our earlier notational setup prevents this from being a problem in the following proof.}
since $0 \leq s \leq R(n) \leq \frac{1}{4}(A_1 + A_3)^{-1}n^{-a_1 - a_3}$,
\[
\left(\frac{3}{4}A_3^{-1}n^{-a_3}\right)p(\theta|x) \leq \left|\frac{d}{dt}p(\theta \mid x + tv)\right|(0) \leq \left(\frac{4}{3}A_3n^{a_3}\right)p(\theta|x).
\]

Applying part (1) of Assumption A.3, recalling $0 \leq s \leq R(n) \leq \frac{1}{4}n^{-2c}$, and using (A.6), this yields
\[
\left(\frac{1}{2}A_3^{-1}n^{-a_3}\right)p(\theta|x) \leq \left|\frac{d}{dt}p(\theta \mid \phi_{x,v}(t))\right|(0) \leq (2A_3n^{a_3})p(\theta|x),
\]
for all sufficiently large $n \in \mathbb{N}$. Note we could have chosen any constant $< 3/4$ for the lower bound and $> 4/3$ for the upper bound, and just selected 1/2 and 2 for convenience. Reparameterizing the previous expression,
\[
\left(\frac{1}{2}A_3^{-1}n^{-a_3}\right)p(\theta|\phi_{x,v}(s)) \leq \left|\frac{d}{dt}p(\theta \mid \phi_{x,v}(t))\right|(s) \leq (2A_3n^{a_3})p(\theta|\phi_{x,v}(s)),
\]
Thus, for all $0 \leq s \leq R(n)$, we have by Gronwall’s inequality
\[
\log\left(\frac{p(\theta|\phi_{x,v}(s))}{p(\theta|\phi_{x,v}(0))}\right) = \log\left(\frac{p(\theta|\phi_{x,v}(s))}{p(\theta|x)}\right) \in \Theta^+(s) \cup \Theta^-(s), \quad (A.11)
\]
where
\[
\Theta^+(s) = \left\{ \theta \in B_1 \cap B_1(v, x) : \frac{1}{2}A_3^{-1}n^{-a_3} \leq s^{-1} \log\left(\frac{p(\theta|\phi_{x,v}(s))}{p(\theta|x)}\right) \leq 2A_3n^{a_3} \right\}
\]
\[
\Theta^-(s) = \left\{ \theta \in B_1 \cap B_1(v, x) : \frac{1}{2}A_3^{-1}n^{-a_3} \leq -s^{-1} \log\left(\frac{p(\theta|\phi_{x,v}(s))}{p(\theta|x)}\right) \leq 2A_3n^{a_3} \right\}.
\]
Applying Inequality (A.11), we have
\[
\|p(\cdot|\phi_{x,v}(s)) - p(\cdot|x)\|_{TV} \geq \int_{\theta \in \Theta^+} |p(\theta|x) - p(\theta|\phi_{x,v}(s))|d\theta
\]
\[
+ \int_{\theta \in \Theta^-} |p(\theta|x) - p(\theta|\phi_{x,v}(s))|d\theta
\]
\[
\geq \left(\frac{e^{\frac{1}{2}A_3^{-1}n^{-a_3}} - 1}{\theta \in \Theta^+} p(\theta|x) + \left(1 - e^{\frac{1}{2}A_3^{-1}n^{-a_3}}\right)\int_{\theta \in \Theta^-} p(\theta|\phi_{x,v}(s))d\theta
\]
\[
\geq e^{\frac{1}{2}A_3^{-1}n^{-a_3}} \left(1 - e^{\frac{1}{2}A_3^{-1}n^{-a_3}}\right)\int_{\theta \in \Theta^+} p(\theta|x) + \left(1 - e^{\frac{1}{2}A_3^{-1}n^{-a_3}}\right)e^{-2A_3sn^{a_3}}\int_{\theta \in \Theta^+} p(\theta|x)d\theta
\]
\[
\geq \left(\frac{e^{-2A_3sn^{a_3}} + e^{\frac{1}{2}A_3^{-1}n^{-a_3}}}{}\left(1 - e^{\frac{1}{2}A_3^{-1}n^{-a_3}}\right)\int_{\theta \in \Theta^+} p(\theta|X)d\theta
\]
\[
\geq \frac{s}{2A_3}n^{-a_3}\int_{\theta \in B_1 \cap B_1(v, x)} p(\theta|X)d\theta
\]
Observe, however, that there is nothing special about the point \( x = \phi_{x,v}(0) \) on the curve \( \{ \phi_{x,v}(s) \} \), except that it is in the middle of the range of values of \( s \) for which \( \phi_{x,v} \) is guaranteed to exist. Thus, by the same calculation, we can conclude that for all \( 0 \leq |s_1|, |s_2| \leq \frac{1}{2} R(n) \),

\[
\| p(\cdot|\phi_{x,v}(s_1)) - p(\cdot|\phi_{x,v}(s_2)) \|_{TV} \geq \frac{|s_1 - s_2|}{10A_3} n^{-a_3}.
\]  

(A.12)

This tells us that for our choice of \((x,v)\), small perturbations of the data \( \phi_{x,v}(s) \in G \) will have quite different posterior distributions for most small values of \( s \).

We now check that, for any distribution \( \pi \), we have

\[
\| p(\cdot|X) - \pi \|_{TV} \geq \frac{S(n)}{160A_3} n^{-a_3-2}
\]

holds w.e.p.

To do this, we will define for \( 0 \leq s \leq \frac{1}{2} R(n) \) a Metropolis-Hastings transition kernel \( Q_s \) with stationary measure equal to \( \tilde{\gamma}_{n,Y} \) conditioned on being in the set \( G(x) \cap E \), which we denote \( \tilde{\gamma}_{n,Y} \). To sample from \( Q_S(x_0, \cdot) \),

1. Sample \( V \sim \text{Unif}(W(x_0)) \) and \( S \sim \text{Unif}([-s, s]) \).
2. Propose the point \( X' = \phi_{x_0,v}(s) \)
3. Accept or reject \( X' \) using the usual Metropolis-Hastings rejection step.

By Assumption 4.1, \( \gamma_{n,Y} \) changes little over small intervals and so the probability of rejection can be made arbitrarily small by choosing a small value of \( s \). More precisely, it implies that there exists some \( 1 < \tilde{a} < \infty \) so that for \( X \sim \tilde{\gamma}_{n,Y} \), the random measure \( Q_{n-\tilde{a}}(X, \cdot) \) has the following property: w.e.p., either the proposed point \( X' \) is accepted or the proposed point is not in \( E \).

Set \( s = s(n) = \min(\frac{1}{2} R(n), n^{-\tilde{a}}) \). Sample \( X \sim \tilde{\gamma}_{n,Y} \), and let \( V, S \) be the additional random variables sampled to construct \( X' \) in the above algorithm for sampling from \( Q_S(X, \cdot) \). We now consider two cases:

1. \( \inf_{-s(n) \leq t \leq s(n)} \| p(\cdot|\phi_{x,v}(t)) - \pi \|_{TV} \geq \frac{s(n)}{480A_3} n^{-a_3-2} \). In particular, choosing \( t = 0 \) gives \( \| p(\cdot|X) - \pi \|_{TV} \geq \frac{s(n)}{480A_3} n^{-a_3-2} \) as well.
2. \( \inf_{-s(n) \leq t \leq s(n)} \| p(\cdot|\phi_{x,v}(t)) - \pi \|_{TV} \leq \frac{s(n)}{480A_3} n^{-a_3-2} \). Although the infimum may not be achieved for any value of \( t \in [-s(n), s(n)] \), there does

\[\text{This Metropolis-Hastings kernel is purely a proof device - it need not be computationally tractable.}\]
always exist some \( s' = s'(X, V) \in [-s(n), s(n)] \) satisfying
\[
\|p(\cdot | \phi_{X,V}(s')) - \pi\|_{TV} \leq 2 \inf_{-s(n) \leq t \leq s(n)} \|p(\cdot | \phi_{X,V}(t)) - \pi\|_{TV}.
\]

When \((X, V)\) is \(\mathfrak{A}\)-good, we have by Inequality (A.12) that for all \(0 \leq t \leq s(n)\),
\[
\|p(\cdot | \phi_{X,V}(t)) - \pi\|_{TV} \geq \|p(\cdot | \phi_{X,V}(t)) - p(\cdot | \phi_{X,V}(s'))\|_{TV} - \|p(\cdot | \phi_{Z,V}(s')) - \pi\|_{TV}
\geq \frac{|t - s'|}{10A_3} n^{-a_3} - \frac{s(n)}{20A_3} n^{-a_3 - 2}.
\]

Since \( S \) was chosen uniformly in \([-s(n), s(n)]\), we have \(\mathbb{P}[|S - s'| \geq n^{-2}s(n)] \geq 1 - n^{-2}\), and so this implies
\[
\mathbb{P} \left( \|p(\cdot | \phi_{X,V}(t)) - \pi\|_{TV} \leq \frac{s(n)}{20A_3} n^{-a_3 - 2} \right) \cap \{(X, V) \text{ is } \mathfrak{A}\text{-good}\} \leq n^{-2}.
\]

Thus, in both cases, \(\{\|p(\cdot | \phi_{X,V}(t)) - \pi\|_{TV} \geq \frac{s(n)}{40A_3} n^{-a_3 - 2}\} \cup \{(X, V) \text{ is not } \mathfrak{A}\text{-good}\}\) holds w.e.p. Since \(\{(X, V) \text{ is } \mathfrak{A}\text{-good}\}\) holds w.e.p. by assumption, we conclude that \(\{\|p(\cdot | \phi_{X,V}(t)) - \pi\|_{TV} \geq \frac{s(n)}{40A_3} n^{-a_3 - 2}\}\) holds w.e.p. \(\square\)

### A.2.2. Application to Exponential Family Regression Models

In this section, we consider exponential family regression models of the form

\[
p((x, y) | \beta, \sigma) = \prod_{i=1}^{n} a(y_i, \sigma) e^{\frac{b(x_i, \beta) - c(x_i, \beta)}{d(\sigma)}}
\]

(A.13)

where \( y_i \in \mathcal{Y} \) is a sample space, \( X_i \in \mathcal{X} \equiv \mathbb{R}^d \) is a sample space for the covariates, \((\sigma, \beta) \in \Theta = [0, \infty) \times \mathbb{R}^d \) is a parameter space, and \( a : \mathcal{Y} \to [0, \infty), b : \mathbb{R} \to \mathbb{R}, c : \mathbb{R} \to \mathbb{R} \) and \( d : \mathbb{R}_+ \to \mathbb{R}_+ \) are further functions. Recall that the logistic regression model (1.5) is a special case.

We now fix a prior \( p \) and data-generating distribution \( \gamma \) for the covariates, and introduce some basic assumptions about models in this class that will be used (along with moderate assumptions about the test statistics being used) to check Assumption A.3. To do so, we need some notation related to the collection of points for which the MLE is fixed.

Throughout, we will assume \( \sigma \) is known. Then, the MLE for a GLM is defined by the equations:

\[
0 = \frac{\partial}{\partial \beta_j} \log p((x, y) | \beta, \sigma) = \sum_{i=1}^{n} x_{ij} \frac{\partial}{\partial \beta_j} \left( \frac{b(x_i, \beta)}{d(\sigma)} \gamma - \frac{\partial}{\partial \beta_j} c(x_i, \beta) \right)
\]

(A.14)

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Denote by \( \hat{\beta} = \hat{\beta}(z_0) \) the point that solves (A.14) for the observed data \( z_0 = (y_0, x_0) \). Let \( f : \mathbb{R}^{np+p} \to \mathbb{R}^p \) be the function of \( x, \beta \) defined by the set of partial derivatives on the right side in (A.14), so that the set of points where the MLE is equal to some particular \( \beta \) is contained in

\[
S(\beta) = \{ x : f(x, \beta) = 0 \},
\]

with \( f_j(x, \beta) = [f(x, \beta)]_j \). Let

\[
f : \mathbb{R}^{np} \to \mathbb{R}^p
\]

be the function of \( x, \beta \) defined by the set of partial derivatives on the right side in (A.14), so that the set of points where the MLE is equal to some particular \( \beta \) is contained in

\[
S(\beta) = \{ x : f(x, \beta) = 0 \},
\]

with \( f_j(x, \beta) = [f(x, \beta)]_j \). Let

\[
J(x, \beta) = \left[ \frac{\partial f_j}{\partial \beta_k}(x, \beta) \right]
\]

be the Jacobian of the map \( f \), with elements

\[
J_{jk}(x, \beta) = \sum_{i=1}^n x_{ij}x_{ik} F(\zeta_i)
\]

For \( 1 \leq i \leq n \), we then define the derivative at \( x_1, \ldots, x_n \):

\[
V_{jk}[i] = \left( \frac{\partial}{\partial \delta} J_{jk}(x_1, \ldots, x_{i-1}, x_i + \delta(1, 1, \ldots, 1), x_{i+1}, \ldots, x_n, \beta) \right)(0)
\]

where \( \alpha = \sum_{j=1}^p \beta_j \) and \((1, 1, \ldots, 1)\) is a vector of ones.

Let \( \mathcal{M} = \{ (i, j) \in \{1, 2, \ldots, p\}^2 : i \leq j \} \) and \( m = |\mathcal{M}| \). Define \( W \) to be the by \( n \times m \) matrix whose \( i \)th row is \( \{V_{\ell}[i]\}_{\ell \in \mathcal{M}} \equiv (W_{i1}, \ldots, W_{im}) \equiv W^{(i)} \). For \( \epsilon > 0 \), \( i \in \{1, 2, \ldots, n\} \), vectors \( x, \xi \in \mathbb{R}^p \) and \( v \in \mathbb{R}^m \) with \( \|\xi\| = \|v\| = 1 \), define

\[
R_v^{(i)}(\epsilon; \xi, x) = \sum_{(j,k) \in \mathcal{M}} [ (x_k + \epsilon \xi_k) F(\zeta + \epsilon \xi') + (x_j + \epsilon \xi_j) F(\zeta + \epsilon \xi') \]

\[
+ (x_j + \epsilon \xi_j) (x_k + \epsilon \xi_k) F''(\zeta + \epsilon \xi') \alpha] v_{jk}
\]

and

\[
\hat{R}_v^{(i)}(\xi, x) = \left( \frac{d}{d\epsilon} R_v^{(i)}(\epsilon; \xi, x) \right)(0),
\]

the directional derivative of \( <W^{(i)}, v> \) with respect to \( x_i \) in the direction \( \xi \).
Assumptions A.5. We make the following assumptions about the GLM, data-generating distribution $\gamma$, and true parameter $\beta_0$:

1. **Good $\gamma$:** Assumption 4.1 holds. Furthermore, the MLE $\hat{\beta}_n$ based on $n$ datapoints satisfies
   \[
   \Pr[\|\hat{\beta}_n - \beta_0\| > \omega_n \text{ infinitely often}] = 0 \quad \text{(A.20)}
   \]
   for some sequence $\lim_{n \to \infty} \omega_n = 0$, where $\beta_0$ is the true parameter value.  

2. **Moderate Growth and Nonsingularity of Functions:** The functions $a, b, c, d$ are smooth. Furthermore, for all $i \in \{1, 2, \ldots, n\}$,
   \[
   \sup_{\|x\| = \|\xi\| = 1} \inf_{\|v\| = 1} |\hat{R}_i(v, x)| > 0. \quad \text{(A.21)}
   \]

3. **Moderate Growth of Data:** Sample $X_1, \ldots, X_n \overset{i.i.d.}{\sim} \gamma$ and $Y_i | X_i \sim p(\cdot | X_i, \beta_0)$. We have
   \[
   \Pr \left[ \max_{1 \leq i \leq n} \frac{\log(\|X_i, Y_i\|)}{\log(n)} = O(1) \right] = 1. \quad \text{(A.22)}
   \]

4. **Anticoncentration of Data:** For fixed $\theta$, define the collection of independent random variables $V_{i,j} = D_{i,j}(X, \theta)$ and define $\rho_{\max}(\theta)$ to be the maximum of the densities of these random variables. We assume that there exists $B_2 \subset \Theta$ and $c, C > 0$ satisfying
   \[
   \sup_{\theta \in B_2} \rho_{\max}(\theta) = n^{O(1)} \quad \text{(A.23)}
   \]
   \[
   \lambda(B_2) \leq Cn^{-c} \quad \beta_0 \in B_2.
   \]

**Remark A.6 (The (Not-So-)Difficult Condition).** As we will see, most of these conditions are straightforward to verify either by inspection of the model or by simple assumptions on the tails of various distributions. The one exception seems to be Inequality (A.21) - while it appears to hold for a wide variety of models (and its analogues appear to hold for a wide variety of control variates), we don’t know a way to verify it in any great generality.

While this makes e.g. Theorem 6 less general than it might otherwise be, there is a straightforward way to use a computer to obtain a certificate that

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12 Notice that for this condition to hold, it is enough for $\hat{\beta}_n \rightarrow \beta_0$ a.s.

13 Note that, in this expression, \(\left\{\frac{\max_{1 \leq i \leq n}(\log(\|X_i, Y_i\|))}{\log(n)}\right\}_{n \in \mathbb{N}}\) is a (random) sequence indexed by $n \in \mathbb{N}$; the event that this sequence is $O(1)$ is exactly the event that this sequence is bounded.

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this condition holds for a particular model of interest. To see this, note that $\hat{R}^{(i)}(\xi, x)$ is an inner product. Thus, for any choice $\xi = \xi^{(1)}, x = x^{(1)}$, the set

$$V^{(1)} = \text{Span}\{v : |\hat{R}^{(i)}(\xi^{(1)}, x^{(1)})| = 0\}$$

is an easily-computed hyperplane; furthermore, it is of codimension 1 unless the coefficients for this inner product all vanish. Continuing to choose points $(\xi^{(2)}, x^{(2)}), \ldots$ and computing $V^{(2)}, V^{(3)}, \ldots$ the same way, we can verify Inequality (A.21) by checking that $\cap_{j=1}^{\ell} V^{(j)} = \{0\}$ for some (finite) $\ell$. We expect that simply sampling $\ell = m + 1$ such pairs uniformly at random will work in most situations.

If we wish to consider a data-generating process for the covariates that does not have full support on e.g. a unit ball, we can run the above algorithm while only choosing pairs $x^{(k)}, \xi^{(k)}$ such that $\{x^{(k)} + s\xi^{(k)}\}_{s=0}^S$ is in the support of the data-generating process for sufficiently small $S > 0$.

We now check Assumption A.5 for several families of GLMs. For any GLM in canonical form, we always have $b(x) = x$. The following are some popular families of GLMs in canonical form:

**Definition A.7.** [Some Common GLMs]

1. logistic regression: $a = 1, c = \log(1 + e^{x_{i}\beta}), d = 1$
2. binomial logistic regression: $a = \binom{n}{y_i}, c = n \log(1 + e^{x_{i}\beta}), d = 1$
3. Poisson regression: $a = (y_i!)^{-1}, c = e^{x_{i}\beta}, d = 1$

**Lemma A.8.** Assume that the prior $p$ has bounded density function and subexponential tails. Then the functions in Definition A.7 satisfy all four conditions of Assumption A.5 as long as they satisfy the first condition. Similarly, the second part of Assumption 4.1 is satisfied as long as $\gamma$ satisfies the first part.

**Proof.** We start with some preliminary calculations:

$$D_{i,j}(\theta, X) = \frac{1}{p(\theta|X)} \frac{\partial}{\partial x_{ij}} p(\theta|X)$$

$$= \frac{1}{p(\theta) \prod_{i=1}^{n} a(y_i, \sigma) e^{b(x_{i}\beta)y_i - c(x_{i}\beta)} d(\sigma)} \frac{\partial}{\partial x_{ij}} \left( p(\theta) \prod_{i=1}^{n} a(y_i, \sigma) e^{b(x_{i}\beta)y_i - c(x_{i}\beta)} d(\sigma) \right)$$

$$= \frac{1}{d(\sigma)} \left\{ \frac{\partial}{\partial x_{ij}} b(x_{i}\beta)y_i - \frac{\partial}{\partial x_{ij}} c(x_{i}\beta) \right\}$$

$$= \frac{\beta_j}{d(\sigma)} \{b'(x_{i}\beta)y_i - c'(x_{i}\beta)\}$$
and

\[ D_{\text{max}}(\theta, X) = \max_{i,j,j',i'} \frac{1}{p(\theta|X)} \left| \frac{\partial^2}{\partial x_{ij} \partial x_{i'j'}} p(\theta|X) \right| \]

\[ = \max_{i,j,j',i'} \frac{1}{d(\sigma)^2} \left\{ \left( \frac{\partial}{\partial x_{ij}} b(x_i \beta)y_i - \frac{\partial}{\partial x_{ij}} c(x_i \beta) \right) \left( \frac{\partial}{\partial x_{i'j'}} b(x_{i'} \beta)y_{i'} - \frac{\partial}{\partial x_{i'j'}} c(x_{i'} \beta) \right) \right\} \]

\[ + 1_{\{i=i'\}} \left( \frac{\partial^2}{\partial x_{ij} \partial x_{ij}} b(x_i \beta)y_i - \frac{\partial^2}{\partial x_{ij} \partial x_{ij}} c(x_i \beta) \right) \]

\[ = \max_{i,j,j',i'} \frac{\beta_j \beta_{j'}}{d(\sigma)^2} \left( \{ b'(x_i \beta)y_i - c'(x_i \beta) \} \{ b'(x_{i'} \beta)y_{i'} - c'(x_{i'} \beta) \} \right) \]

\[ + 1_{\{i=i'\}} \left\{ b''(x_i \beta)y_i - c''(x_i \beta) \right\} \).

We now check the parts of Assumption A.5 in order:

1. This is assumed.
2. The first part of the condition is clear by inspection. To verify Inequality (A.21), we start by restricting our attention to vectors \( \xi \) that satisfy \( \xi^\prime \beta = 0 \). In that case, considering the vector \( \xi \propto \beta \) immediately allows you to see that the first derivative is not also identically 0 in this case.
3. Inequality (A.22) follows almost immediately from the fact that the prior \( p \), the covariate-generating distribution \( \gamma \), and the model likelihoods all have subexponential tails.

More carefully: since \( \gamma \) and \( p \) have subexponential tails, there exists some 0 < \( A < \infty \) such that, for \( \theta \sim p \) and \( X_1, \ldots, X_n \sim \gamma \),

\[ \mathbb{P}[\max(||\theta||, \max_{1 \leq i \leq n} ||X_i||) > A \log(n)] \leq n^{-3}. \] (A.25)

In the two logistic regression cases, \( Y_i \leq n \) deterministically. In the remaining case, define the random quantity \( A_{\text{max}} = \max(||\theta||, \max_{1 \leq i \leq n} ||X_i||) \); typical concentration inequalities for subexponential random variables

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tell us $P[\max_{1 \leq i \leq n} |Y_i| > (A_{\text{max}}^2 + 1) \log(n)] \leq n^{-3}$ for all $n$ sufficiently large.\(^{14}\) Combining these two bounds on $\max_{1 \leq i \leq n} |Y_i|$ with Inequality (A.25) completes the proof.

(4) We have explicit formulas for $D_{ij}$ and its arguments; the claim can be verified by seeing that none of these formulas have super-polynomially large values outside of $O(n)$ singularities.

Finally, we verify the second part of Assumption 4.1. In any generalized linear model in canonical form, the ratio of densities

$$
\frac{g_{n,y}(X)}{g_{n,y}(\tilde{X})}
$$

can be written in the form

$$
\frac{g_{n,y}(X)}{g_{n,y}(\tilde{X})} = H(X, \tilde{X}) e^{-(X-\tilde{X})'y}
$$

for some function $H$ that does not depend on $y$. Thus, as long as there exists a constant $c$ such that $\|Y\| < n^c$ w.e.p, then we can choose $d_1, d_2$ such that the second part of Assumption 4.1 holds whenever the first part holds. \(\square\)

Finally, we check that Assumption A.5 implies Assumptions A.3 for reasonable test statistics:

**Lemma A.9.** Consider a GLM model that satisfies Assumption A.5, along with test statistics $T_1, \ldots, T_d$ as in the statement of Theorem 6. Then Assumption A.3 is also satisfied.

**Proof.** We consider the three parts of Assumption A.3 in order; the first is by far the longest.

**First Condition:** Let $S$ be as in Equation (A.15), and assume the Jacobian $J$ defined in Equation (A.16) is invertible at some $x \in S(\hat{\beta})$. By the implicit function theorem, there exists an open set $U = U(x) \subset \mathbb{R}^{np}$ containing $x$ and a continuously differentiable function $g : U \to \mathbb{R}^p$ such that

$$
g(x') = \hat{\beta}
$$

and

$$
f(x', g(x')) = 0
$$

for all $x' \in U$, and furthermore with

$$
\left( \frac{\partial g}{\partial x_{ij}} \right)(x') = -J^{-1}(x', \hat{\beta}) \left( \frac{\partial f}{\partial x_{ij}} \right)(x', g(x')).
$$

\(^{14}\)This bound is extremely conservative.
We will need to verify that $U$ contains a ball of radius $n^{-O(1)}$ and the smallest singular value $\sigma(J)$ of $J$ is $n^{-O(1)}$, at least at most such points $x$. To do this, we will need a new bound on the smallest singular value of a random matrix that is stated and proved in Appendix B. In particular, we will verify the assumptions of Lemma B.1 to bound the smallest singular value of $J$, then invoke the quantitative version of the implicit function theorem found in [Phi12] to bound the size of $U$. We now set up the notation required to verify the assumptions of Lemma B.1, following the notation for that lemma closely.

Inequality (A.21) (and the Assumption 4.1 that $\gamma$ has nonzero density on the unit ball) immediately implies that conditions (B.1) and (B.2) of Lemma B.1 are satisfied. Condition (B.3) of Lemma B.1 follows immediately from the assumption that the functions $a,b,c,d$ in the definition of the GLM are smooth and the support of the covariates is compact. Applying Lemma B.1, we conclude that there exists $\eta > 0$ so that

$$\{\sigma(J(X,\beta)) \geq \eta\}$$

holds w.e.p. for any fixed $\beta$, including $\beta_0$. Since $\|\hat{\beta} - \beta_0\| = o(1)$ w.e.p. by Inequality (A.20), and $J(\cdot, \beta)$ is a continuous function of $\beta$, this implies that there exists a constant $\eta'$ such that

$$\{\sigma(J(X,\hat{\beta})) \geq \eta'\}$$

holds w.e.p. Applying the main result of [Phi12] with the same bounds on the derivatives of $J$ gives the desired result.

**Second Condition:** We see that Inequality (A.7) holds w.e.p. whenever $a,b,c,d$ are smooth, $\gamma$ has bounded support and Inequality (A.22) holds. Inequalities (A.8) and (A.9) follow from an application of Lemma C.1, with bound on $\rho_{\max}$ coming from Inequality (A.23).

**Third Condition:** We can see by inspection that the derivatives of $p$ are polynomially bounded in all arguments; the arguments themselves are polynomially bounded w.e.p. by the fact that $a,b,c,d$ are smooth, the fact that $\gamma$ has compact support, and Inequality (A.22).

$\Box$

### A.3. Proof of Theorem 6.

**Proof of Theorem 6.** By our assumption on $\gamma$ and the usual strong consistency theorem for the MLE $^{15}$, the first part of Assumption A.5 is satisfied. By

---

$^{15}$See e.g. Theorem 2 of [FK+85]. Most of the conditions can be verified immediately, so we give short details only for one of them: Condition $(S_\delta)$ clearly holds when all variables in the Fisher information matrix are replaced by their expectation; application of Hoeffding’s inequality for i.i.d. bounded random variables then implies that $(S_\delta)$ itself holds.
Lemma A.8, the remaining parts of Assumption A.5 and all parts of Assumption 4.1 are also satisfied. This means that, by Lemma A.9, Assumptions A.3 are satisfied. The result then follows immediately: the warm start condition follows from Lemma A.1 (as well as the usual Bernstein-von Mises theorem showing convergence of the rescaled posterior), and the remaining conditions follow from applying Lemma A.4 (whose conditions are satisfied because Assumptions A.3 are satisfied).

□

Appendix B. Bounds on Singular Values of Structured Random Matrices

In this section, we give a simple generic bound on the smallest singular value of a very special class of random matrices with highly dependent entries. These can be applied to show that the manifolds \( \mathcal{G}(x) \) defined in (A.4) will typically have inner curvature that is not too close to 0. The variables defined in this section use notation that is independent of the rest of the paper, though we have tried to make it look similar.

For a generic square matrix \( A \), we denote by \( \sigma(A) \) its smallest singular value. For a generic \( p \times q \) matrix \( A \) with \( p < q \) and \( I \subset \{1,2,\ldots,q\} \), we denote by \( \sigma_{\text{maximin}}(A) = \max_{I \subset \{1,2,\ldots,q\}} |I| = p \sigma(A_I) \) the largest value of the smallest singular values of all square \( p \times p \) submatrices.

We denote by \( M \) a \( p \) by \( p \) matrix, and we write each entry \( M_{ij} = M_{ij}(x_1,\ldots,x_n) \equiv \sum_{k=1}^n m_{ijk}(x_k) \) as an additive function of points \( x_1,\ldots,x_n \in \mathbb{R}^d \). Next, define the set \( \mathcal{M} \) to be either \( \{1,2,\ldots,p\}^2 \) when \( M \) is not symmetric or \( \{(i,j) \in \{1,2,\ldots,p\}^2 : i \leq j\} \) when \( M \) is symmetric. In either case we let \( m = |\mathcal{M}| \).

We then define derivatives: let

\[
W_{ij}^{(k)}(x_1,\ldots,x_n) = \left( \frac{d}{d\delta} M_{ij}(x_1,\ldots,x_{k-1},x_k + \delta(1,1,\ldots,1),x_{k+1},\ldots,x_n) \right)(0) = \left( \frac{d}{d\delta} m_{ijk}(x_k + \delta(1,1,\ldots,1)) \right)(0);
\]

note that, as \( x_k \) is a vector, this last expression is generally not equal to \( m_{ijk}^{(s)}(x_k) \).

Finally, for \( s \in \mathbb{N} \), \( \xi \in \mathbb{R}^m \) and \( v \in \mathbb{R}^m \), define

\[
R_v^{(k)}(\xi,s;x) = \left( \frac{d^s}{d\delta^s} \sum_{(i,j) \in \mathcal{M}} W_{ij}^{(k)}(x_1,\ldots,x_{k-1},x_k + \delta\xi,x_{k+1},\ldots,x_n)v_{ij} \right)(0).
\]
Lemma B.1. Fix an interval $I \subset \mathbb{R}$. Assume that there exists some $\mathcal{H} \subset I^p$, an integer $1 \leq S < \infty$ and $a > 0$ so that, for all $v \in \mathbb{R}^m$ and all $k \in \{1, 2, \ldots, n\}$,

$$\sup_{\xi \in \mathbb{R}^p} \sup_{s \in \{1, \ldots, S\}} |R_v^{(k)}(\xi, s; x)| > a$$

(B.1)

at all points $x$ with $x_k \in \mathcal{H}$. Let $X_1, \ldots, X_n$ be independent (but not necessarily identically distributed) random variables drawn from $I^n$, with densities bounded by $A^{-1}$ and $A$, and assume that

$$\min_i \mathbb{P}[X_i \in \mathcal{H}] > 0.$$  

(B.2)

Furthermore, assume

$$\sup_{x_1, \ldots, x_n \in I} \max_{k, k', i, j} \left| \frac{\partial^2}{\partial x_{k\ell} \partial x_{k'\ell'}} M_{ij}(x_1, \ldots, x_n) \right| < \infty.$$  

(B.3)

Then there exists $c > 0$ depending only on $A, p, a, S, I, \mathcal{H}$ and the values of the expressions (B.2), (B.3) so that the random matrix $M = M(X_1, \ldots, X_n)$ satisfies

$$\{\sigma(M) > c\}$$

w.e.p.

Proof. By Inequalities (B.1) and (B.2), there exist constants $\eta, \epsilon > 0$ so that for all $v \in \mathbb{R}^m$ with $\|v\| = 1$ and all $k \in \{1, 2, \ldots, n\}$,

$$\mathbb{P}[|\sum_{\ell \in M} W_{\ell}^{(k)} v_\ell| < \eta] < 1 - \epsilon.$$

Observing that the rows $W^{(1)}, \ldots, W^{(n)}$ of $W$ are independent, this implies that for any $I \subset \{1, 2, \ldots, n\}$,

$$\sup_{\|v\| = 1} \mathbb{P}\left[ \max_{i \in I} |\langle W^{(i)}, v \rangle| < \eta \right] \leq (1 - \epsilon)^{|I|}.$$

We can thus choose a sequence $i_1 = 1, i_2 \in \{\frac{n}{m} + 1, \ldots, \frac{2n}{m}\}, \ldots, i_m \in \{\frac{n(m-1)}{m}, \ldots, n\}$ so that, applying the previous inequality and taking a union bound,

$$\mathbb{P}\left[ \min_{1 \leq q \leq p} d(W^{(i_q)}, \text{Span}(\{W^{(i_{q'})}\}_{q' \neq q})) < \eta \right] \leq m(1 - \epsilon)^{\frac{n}{m} - 1},$$

where $d(w, H)$ denotes the usual distance between a vector $w$ and hyperplane $H$.

Applying Lemma 1.11 of [Cha], this means

$$\mathbb{P}[\sigma_{\text{maximin}}(W) < \eta] \leq m(1 - \epsilon)^{\frac{n}{m}}.$$  

(B.4)
On the event \( \{ \sigma_{\text{maximin}}(W) < \eta \} \), for every vector \( w \) of norm \( \| w \| = 1 \) we can find a solution to
\[
W \Delta = w
\]
with norm
\[
\| \Delta \| = O(m \eta^{-1}). \tag{B.5}
\]

For \( i \in \mathcal{M} \), denote by \( w^{(i)} \) the \{0, 1\}-valued vector with a single 1 at index \( i \). For \( \alpha > 0 \), denote by \( \mathcal{SC}(\alpha) \) the collection of probability measures \( \pi \) on \( \mathbb{R} \) with the property that \( \pi(L) > \alpha \) for some interval \( L \) of length \( |L| < \alpha \).

We will now apply Lemma C.4, stated in the section. We verify the assumptions in that lemma. The bound on \( A \) is given by assumption, the bound on \( B \) is given by Inequality (B.5) applied to the vector \( w^{(i)} \), the bound on \( C \) given by Inequality (B.3), and the bound on the probability of \( \mathcal{J}_{1} \) (and hence \( \mathcal{J}_{2} = \mathcal{J}_{1} \)) given by Inequality (B.4). By Lemma C.4, there exists some \( \eta'' > 0 \) not depending on \( n \) so that for all \( 1 \leq i \leq p \), the conditional distribution \( \mathcal{L}(M_{ii} | \{ M_{jk} \}_{(j,k) \neq (i,i)}) \) satisfies event
\[
\mathbb{P}[\mathcal{L}(M_{ii} | \{ M_{jk} \}_{(j,k) \neq (i,i)}) \in \mathcal{SC}(\eta'')] = e^{-\Omega(\frac{\eta''}{n})}, \tag{B.6}
\]
where in this probability statement we view the randomness as coming from the collection \( \{ M_{jk} \}_{(j,k) \neq (i,i)} \), which are functions of the random variables \( X_1, \ldots, X_n \).  

Applying the main result of [FG13], this implies that there exists some \( \eta'' > 0 \) also not depending on \( n \) so that
\[
\mathbb{P}[\sigma(M) \geq \eta''] \geq 1 - e^{-\Omega(\frac{\eta''}{n})}, \tag{B.7}
\]
completing the proof.  

\[\square\]

**Appendix C. Anti-Concentration Bounds**

We give several simple anti-concentration bounds.

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16Since we are conditioning on \( \{ M_{jk} \}_{(j,k) \neq (i,i)} \) here, this distribution is not directly parameterized by \( x_1, \ldots, x_n \) as in the statement of Lemma C.4. This can be fixed by locally reparameterizing \( M_{j,k} \) to express it as a linear function on some small domain. As discussed in Remark C.6 immediately following Lemma C.4, by the quantitative version of the implicit function theorem given in [Phi12], there exists such a reparameterization of the form required by Lemma C.4 on a sufficiently large region of \( I^n \); the above bounds on derivatives of \( M_{j,k} = M_{j,k}(x_1, \ldots, x_n) \) are exactly those required by [Phi12].

17As stated, the main result of [FG13] requires that the entry \( M_{ii} \notin \mathcal{SC}(\eta') \) and independent of the random variables \( \{ M_{jk} \}_{(j,k) \neq (i,i)} \). However, inspecting the proof, we see that it only uses the fact that the conditional distribution \( \mathcal{L}(M_{ii} | \{ M_{jk} \}_{(j,k) \neq (i,i)}) \notin \mathcal{SC}(\eta') \).
C.1. Anticoncentration for Sums. We introduce one piece of notation: for \( \epsilon > 0 \), define \( \mathcal{I}_\epsilon \) to be the collection of intervals of length less than \( \epsilon \). We have:

**Lemma C.1.** Let \( X_1, \ldots, X_m \) be a sequence of independent (but not necessarily i.i.d.) random variables with densities uniformly bounded by \( 0 < \rho_{\text{max}} < \infty \), and let \( v \in \mathbb{R}^d \) a vector with norm \( \|v\| = 1 \). Then for any \( \epsilon > 0 \),

\[
\sup_{I \in \mathcal{I}_\epsilon} \mathbb{P} \left[ \sum_{i=1}^m v_i X_i \in I \right] \leq \rho_{\text{max}} \epsilon \sqrt{m}.
\]

**Proof.** Since \( \|v\| = 1 \), there exists some \( i \in \{1, 2, \ldots, m\} \) satisfying \( |v_i| \geq \frac{1}{\sqrt{m}} \). Assume WLOG that this \( i = 1 \). Denote by \( \mathcal{F} \) the \( \sigma \)-algebra generated by \( X_2, \ldots, X_m \). We then have

\[
\sup_{I \in \mathcal{I}_\epsilon} \mathbb{P} \left[ \sum_{i=1}^m v_i X_i \in I \right] = \sup_{I \in \mathcal{I}_\epsilon} \mathbb{E} \left[ \mathbb{P} \left[ \sum_{i=1}^m v_i X_i \in I | \mathcal{F} \right] \right]
\]

\[
\leq \mathbb{E} \left[ \sup_{I \in \mathcal{I}_\epsilon} \mathbb{P} \left[ \sum_{i=1}^m v_i X_i \in I | \mathcal{F} \right] \right]
\]

\[
= \sup_{I \in \mathcal{I}_\epsilon} \mathbb{P} [v_1 X_1 \in I]
\]

\[
\leq \sup_{I \in \mathcal{I}_\epsilon} \mathbb{P} [X_1 \in I]
\]

\[
\leq \rho_{\text{max}} \epsilon \sqrt{m},
\]

where the last line we use the fact that \( X_1 \) is a random variable whose PDF has density bounded by \( \rho_{\text{max}} \). This completes the proof. \( \square \)

C.2. Anticoncentration for Functions. We give an immediate generalization of Lemma 1.2 [Cha19], then apply it to obtain a simple anticoncentration result for functions of many random variables. As Chatterjee writes of Lemma 1.2 of [Cha19], we suspect that both of these are fundamentally well-known results.

**Lemma C.2.** Let \( Y_1, \ldots, Y_k \) be random variables with the same distribution \( \mu \) on \( \mathbb{R} \). Assume that

\[
\mathbb{P} \left[ \min_{1 \leq i < j \leq k} |Y_i - Y_j| \geq \epsilon \right] \geq 1 - \delta \quad (C.1)
\]

for some \( \epsilon, \delta > 0 \). Then for all \( a \in \mathbb{R} \),

\[
\mathbb{P} [Y_1 \in (a, a + \epsilon)] \leq \delta + \frac{1}{k}.
\]
Remark C.3. To use this theorem efficiently, the random variables $Y_1, \ldots, Y_k$ should usually not be independent. We note that this result can be generalized to variables with slightly different distributions, as in [Cha19], but this is beyond the scope of the current article.

Proof. The argument is essentially identical to Lemma 1.2 [Cha19]: we simply note that either the rare event whose probability is bounded in Inequality (C.1) occurs, or at most one of $Y_1, \ldots, Y_k$ is in the interval $(a, a + \epsilon)$. \hfill \Box

We next give a quick consequence that says, roughly: if $Y = F(X_1, \ldots, X_n)$ is a function of many independent random variables, and the first derivatives of $F$ is not always very small, and the second derivatives of $F$ are never very large, then $Y$ cannot be concentrated on any small interval. The statement of the lemma is more complicated than this primarily because we wish to allow the bounds on the derivatives to fail on certain exceptional sets.

Lemma C.4. Fix constants $A, B, C, D > 0$ and $m, k \in \mathbb{N}$ and a $C^2$ function $F : [0, 1]^n \mapsto \mathbb{R}$. Denote by $J_1 = \{x \in [0, 1]^n : \sup_{v \in \mathbb{R}^n : \|v\| = 1} |(\nabla_v F)(x)| \geq B\}$ the set of points for which the derivative is large in some direction; for $x \in J_1$, let $v = v(x)$ be the vector achieving the supremum in the condition. Next, let $J_2 = \{x \in J_1 : \sup_{y : \|x - y\| \leq D} \|H(F)(y)\|_{\infty} \leq C\}$, where $H(F)$ denotes the usual Hessian of $F$, the set of points for which the Hessian is not too large. Finally, let $X_1, \ldots, X_n$ be a sequence of independent random variables with densities that are all bounded above by $A$. Then for all $\eta > 0$ and integers $k, m$ satisfying $2km^{-1} \leq \min(\frac{B}{2AC}, \frac{1}{\eta}, D)$,

$$\sup_{s \in \mathbb{R}} \mathbb{P}[|F(X_1, \ldots, X_n) - s| < \frac{B}{2Am}] \leq \frac{1}{k} \left(1 + \prod_{i=1}^n (1 - \frac{2k}{m}|v_i(X_1, \ldots, X_n)|)\right)$$

$$+ \mathbb{P}[\max_i v_i(X_1, \ldots, X_n) > \eta] + \mathbb{P}((X_1, \ldots, X_n) \notin J_2).$$

Remark C.5. We note that, if $A, B, C, D$ are all $n^{-O(1)}$, then we can choose $m, k$ so that the bound $\frac{B}{2Am}$ and the first three terms on the right-hand side of (C.2) are all $n^{-O(1)}$. We will always use the theorem in this qualitative way, but keep the above quantitative version in case it is of independent interest.

Proof. Write $X_i = f_i(U_i)$, where $U_1, \ldots, U_n$ are i.i.d. Unif$[0, 1]$ random variables and $f_i$ is the inverse of the CDF of $X_i$. In the following, we consider only the case that $(X_1, \ldots, X_n) \in J_2$ and $\max_i v_i(X_1, \ldots, X_n) \leq \eta$; we will then try to obtain a bound of the form given by the first two terms in Inequality (C.2).

For $a \in [-1, 1]$ define $\tilde{U}_i[a] = U_i + av_i$ modulo 1. Let $Y = F(X_1, \ldots, X_n)$ and $\tilde{Y}[a] = F(f_1(\tilde{U}_1[a]), \ldots, f_n(\tilde{U}_n[a]))$. Note that $\tilde{U}_i$ are still i.i.d. Unif$[0, 1]$
random variables, and so \( \tilde{Y}[a] \) has the same distribution as \( Y \) for every fixed \( a \). Furthermore, \( \tilde{Y}[0] = Y \).

Next, consider \( 0 \leq a < b \). As long as \( 0 \leq U_i + av_i \leq 1 \) for all \( i \in \{1, 2, \ldots, n\} \),
\[
|\tilde{Y}[a] - \tilde{Y}[b] - (a - b) \nabla_v F(f_1(\tilde{U}_1[a]), \ldots, f_n(\tilde{U}_n[a]))| \leq C(a - b)^2.
\]
When this occurs,
\[
|\tilde{Y}[a] - \tilde{Y}[b]| \geq (a - b) \frac{B}{A} - C(a - b)^2
\]
\[
\geq (\frac{B}{A} - C(a - b))(a - b),
\]
and so for \( (a - b) \leq \frac{B}{2AC} \),
\[
|\tilde{Y}[a] - \tilde{Y}[b]| \geq \frac{B}{2A}(a - b).
\]
Thus, for any integers \( k, m \) satisfying \( 2km^{-1} \leq \frac{B}{2AC} \), we can couple the \( (k + 1) \) random variables \( \tilde{Y}[0], \tilde{Y}[(-k + 1)m^{-1}], \ldots, \tilde{Y}[km^{-1}] \) so that
\[
\mathbb{P}[ \min |\tilde{Y}[p] - \tilde{Y}[q]| \leq \frac{B}{2Am} ] \leq 1 - \mathbb{P}[0 \leq U_i \pm \frac{k}{m}v_i \leq 1] \leq 1 - \prod_{i=1}^{n}(1 - 2\frac{k}{m}|v_i|)
\]
The result then follows from an application of Lemma C.2.

\[\Box\]

**Remark C.6.** We combine this lemma with a quantitative versions of the implicit function theorem (e.g. [Phi12]) to apply this bound for conditioned random variables. More precisely, we consider the case where \( Y = F(X_1, \ldots, X_n) \), and we wish to condition on the values of several other random variables \( H_i(X_1, \ldots, X_n) = c_i \) of the same form, for \( i \in \{1, 2, \ldots, \ell\} \). The implicit function theorem tells us that, under certain conditions, we can find a local parameterization of the space \( \{(x_1, \ldots, x_n) : H_i(x_1, \ldots, x_n) = c_i \forall 1 \leq i \leq \ell\} \) of the form \( \tilde{F} : \mathbb{R}^{n-\ell} \to \mathbb{R} \). When this is possible, we can express the conditioned random variable \( \tilde{Y} \) as a function \( \tilde{F}(\tilde{X}_1, \ldots, \tilde{X}_{n-\ell}) \) for which Lemma C.4 applies. Furthermore, the same bounds on derivatives that appear in the statement of the lemma are sufficient to apply [Phi12].

**Appendix D. Alternative Construction**

In this section, we present and analyze an alternative construction of the Markov chain from Algorithm 1. We first need a short technical lemma. Fix a subset \( S = \{1, 2, \ldots, n\} \) and integer \( k \in \mathbb{N} \), and let \( \ell = \lfloor \frac{n}{k} \rfloor \). Let
$Y[1], Y[2], \ldots, Y[\ell]$ be defined recursively by sampling $Y[1] \sim C_k(S)$ and then according to the following rule:

$$Y[i] \sim C_k(S \setminus \cup_{j=1}^{i-1} Y[j]).$$

Let $\tau$ be any stopping time for this sequence, let $\mu$ be the distribution of the sequence $Y \equiv (Y[1], Y[2], \ldots, Y[\tau])$, and for any $t$ let $M(Y, t) = \cup_{i=1}^{t} \{Y[i]\}$.

**Lemma D.1.** Let $(Y_1, \tau_1), (Y_2, \tau_2), \ldots$ be an adapted sequence with $Y_i \sim \mu_{\tau_j}$. It is possible to couple this sequence to a permutation $\sigma \sim \text{Unif}[S_n]$ such that

$$\cup_{i=1}^{t} M(Y_i, \tau_i) = \{1, 2, \ldots, \max(\sigma(\cup_{i=1}^{t} M(Y_i, \tau_i)))\}$$

for all $I \in \mathbb{N}$.

**Proof.** The permutation $\sigma$ is obtained by just ordering the elements of the subsample as they arrive.

More formally, put each subsample $Y_i$ in an arbitrary order $Y_i = (Y_i(1), \ldots, Y_i(\tau_i))$. Concatenate these to the sequence $(Z_1, Z_2, \ldots) = (Y_1(1), \ldots, Y_1(\tau_1), Y_2(1), \ldots)$. We then define $\sigma$ by initially setting $\sigma^{-1}(1) = Z_1$ and then inductively

$$\sigma^{-1}(j + 1) = Z_{\min\{i : Z_i \notin \{\sigma^{-1}(1), \ldots, \sigma^{-1}(j)\}\}}.$$

$\square$

We are now ready to prove Proposition 5.2:

**Proof of Proposition 5.2.** We note that the observed minibatches in Algorithm 1 are of exactly the form studied in Lemma D.1. Thus, by applying the random permutation $\sigma$ guaranteed by this lemma before running the algorithm, we can obtain a representation for which the datapoints in the interval $(m, n]$ are guaranteed to be used after all of the datapoints in $[1, m]$.

Thus, it remains only to bound the number of steps required to use $m$ out of $n$ datapoints. By standard concentration bounds, the average number of draws per step in any time interval of fixed length $T = \Theta(n \log(n))$ is $O(\exp(\lambda))$, with high probability. Thus, it is sufficient to check that $\Omega(n \log(n))$ draws are required with high probability. But this is exactly what is bounded by the usual coupon-collector bound on the time it takes to collect $m$ coupons when collecting $k$ at a time$^{18}$.

$^{18}$This follows immediately from the classical coupon-collector bound on the time to collect $m$ coupons when collecting 1 at a time, as in [Erd61]. Alternatively, see Lemma D.2 below for a much more general restatement.
We next prove Proposition 5.4, which is rather similar. We will use the following simple variant on the well-known coupon collector problem, which is restated for completeness.

**Lemma D.2.** Fix constants $1 \leq A < \infty$, $k \in \mathbb{N}$ and a function $w : \mathbb{N} \mapsto \left[A^{-1}, A\right]$. For fixed $n \geq k$, define the measure $\mu_n$ on size-$k$ subsets of $\{1, 2, \ldots, n\}$ by

$$\mu_n(\{y_1, \ldots, y_k\}) \propto \prod_{i=1}^{k} w(y_i).$$

Let $Y_1^{(n)}, Y_2^{(n)}, \ldots \overset{i.i.d.}{\sim} \mu_n$ and $Z_j^{(n)} = \bigcup_{i=1}^{j} Y_i^{(j)}$.

Define

$$T_{n,m} = \min\{j : |Z_j^{(n)}| \geq m\}$$

and

$$S_{n,m} = Z_{T_{n,m} - 1}^{(n)}.$$

Then

$$\frac{1}{3} A^{-2} n \log(n) \leq T_{n,n} \leq 3 A^2 n \log(n) \quad (D.1)$$

w.p., and furthermore for fixed $m$ there exists $C_2 < \infty$ so that

$$\sup_{y \subset \{1, 2, \ldots, n\}, |y| = m} \mathbb{P}[y \subset S_{n,m}] \geq C_2 n^{-m} A^{-8mA^4 \log(n)}. \quad (D.2)$$

**Proof.** Inequality (D.1) follows from the same argument as the usual coupon-collector bound found in e.g. the original article [Erd61].

To prove Inequality (D.2), consider any sequence of draws $Y^{(n)} = (Y_1^{(n)}, Y_2^{(n)}, \ldots, Y_{T_{n,m} - 1}^{(n)})$ as in the statement of Lemma D.2, denote by $\eta_n$ the distribution of $Y^{(n)}$. Next, sample $(\hat{y}_1, \ldots, \hat{y}_m) \sim C_m(\{1, 2, \ldots, n\})$, and consider the sequence $\hat{Y}^{(n)} = (\hat{Y}_1^{(n)}, \hat{Y}_2^{(n)}, \ldots, \hat{Y}_{T_{n,m} - 1}^{(n)})$ obtained from $Y$ by *swapping* $y_i$ and $\hat{y}_i$ whenever they appear.

We next bound the ratio $\frac{\eta_n(Y^{(n)})}{\eta_n(\hat{Y}^{(n)})}$. First, note that each substitution decreases the likelihood by at most a factor of $A^2$. Next, note that (by Hoeffding’s inequality combined with Inequality (D.1)), w.e.p. no individual entry $\hat{y}_i$ occurs more than $4A^4n \log(n)$ times. Combining these two facts, we have

$$\frac{\eta_n(Y^{(n)})}{\eta_n(\hat{Y}^{(n)})} \geq A^{-8mA^4 \log(n)}$$

w.e.p. This implies Inequality (D.2).
We then have:

Proof of Proposition 5.4. As with the proof of Proposition 5.2, the bound on the number of steps required to use \( m \) out of \( n \) datapoints follows from the usual coupon-collector argument; the particular version of this bound we need is restated as Inequality (D.1) of Lemma D.2 above.

Inequality (D.2) tells us that the uniform measure on size-\((n-m)\) subsets and the measure on last-\((n-m)\)-points-seen are within a factor of \( A^{-8(n-m)A^4 \log(n)} \) in separation distance. But Inequality (5.5) exactly tells us that large fluctuations still happen w.e.p., even with this factor of \( A^{-8(n-m)A^4 \log(n)} \).

Appendix E. Grid-Based Control Variates

Adding “extra” control variates will typically make Assumptions 2.4 and 2.10 easier to verify with good constants, at the cost of making the constants in Assumption 2.2 worse. In this section we introduce a collection of control variates that we have found to be extremely useful in improving 2.4 and 2.10, and which never substantially worsen the bounds on Assumption 2.2 obtained in Section A.2. See Remark 2.11 for an example in which these control variates are useful.

The construction is simple. Fix a constant \( a \in \mathbb{R} \), let \( \Lambda_{n,a} = \{(j_1 n^{-a}, \ldots, j_d n^{-a})\}_{j_1, \ldots, j_d \in \mathbb{Z}} \), and define the \( i \)’th control variate

\[
T_i(x) = \arg\min_{y \in \Lambda_{n,a}} \|x - y\|,
\]

breaking ties arbitrarily. In other words, \( T_i \) breaks up the state space of the data into polynomially-small boxes, and identifies which box a datapoint is in.

We observe that adding \( T_1, \ldots, T_n \) to a collection of control variates that satisfy Assumption A.2 with constant \( c > 0 \) will result in a new collection of control variates that satisfy Assumption A.2 with some constant that is strictly greater than 0, w.e.p. Since Assumption A.2 is the only place that control variates are used in Section A.2, the remaining arguments go through without modification.

Having shown that these new control variates can easily be incorporated without our earlier arguments breaking down, we give an informal sketch of why this might be useful. As mentioned in Remark 2.11, these control variates decrease the sensitivity of subsamples to the full dataset. While a full discussion is beyond the scope of the present paper, these control variates can also be extremely useful for verifying Assumptions 2.4 and 2.10 with good constants for generic subsampling kernels \( K \) with complicated but smooth control variates.
We sketch such an application. Any $C^1$ control variate $T(x)$ can be estimated by an approximate version $\hat{T}$ according to the formula

$$\hat{T}(x) = T(T_1(x_1), \ldots, T_n(x_n)),$$

with error $\sup_x \|\hat{T}(x) - T(x)\| = O(n^{-a+1})$ when $T$ has uniformly bounded derivatives. This natural leads to an approximate subsampling kernel $\hat{K}$, obtained by replacing $T$ with $\hat{T}$ wherever it appears in the definition of $K$.\footnote{This “definition” of $\hat{K}$ of course depends on the particular presentation of a subsampling algorithm. Naively applying this to all precomputed quantities appearing in the published presentation seems to work well in many examples, including Algorithm 7 of [BDH17b] and the main algorithm of [MA14].}

When $K$ and $\hat{K}$ are sufficiently close, satisfying an inequality of the form

$$d(K, \hat{K}) \ll \min(f(K), f(\hat{K})) \quad \text{(E.2)}$$

for some notion of distance $d$ and mixing rate $f$, standard perturbation theory for Markov chains (see e.g. [AFEB16]) implies that the two transition kernels must have spectral gaps $\lambda(K), \lambda(\hat{K})$ satisfying

$$\frac{\lambda(K)}{\lambda(\hat{K})} \in [0.5, 2]. \quad \text{(E.3)}$$

To conclude: it is straightforward to verify that $T_1, \ldots, T_n$ satisfy Assumption A.2 (and thus often Assumption 2.2) when using the arguments in Section A.2. In some situations, it is straightforward to verify (E.2). When both of these hold, we may apply our main result, Theorem 3, to bound the spectral gap of $\hat{K}$, and then Inequality (E.3) to conclude that a very similar bound holds for $K$. The main advantage of this approach is that Assumption 2.10 may hold for $\hat{K}$ with very large values of $s(n)$, even when it holds only for very small values of $s(n)$ for $K$.

This approach might feel like cheating - if $a$ is large, we are essentially using the original data! Indeed, using a large value of $a$ does cause problems - but these problems appear in the interpretation of the final result. In applying Theorem 3 (for exact chains, such as [MA14]), choosing even very large values of $a$ does not change the interpretation - these new control variates are purely a technical aid. In applying Theorem 5 (for approximate chains, such as many in [BDH17b]), large values of $a$ may change Inequality (3.4). In particular, if $a$ is too large, our main result just gives the (obvious) conclusion that the complete set of control variates essentially determines the posterior.

Thus, using this grid approximation trick requires us to choose a value of $a$ that is large enough to be useful, but small enough to not determine the posterior distribution. To give a very rough illustration: for approximately
normal posterior distributions and algorithms that already use the posterior MLE and the Hessian at the MLE as control variates, we suspect that any choice of $a \leq 1$ will have a small impact on Inequality (3.4) and any choice of $a > 1$ will have a substantial impact.