

# Calibrated Data Augmentation for Scalable Markov Chain Monte Carlo

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**Abstract:** There has been considerable interests in making Bayesian inference more scalable. While most literature focuses on reducing the computing time per iteration, little has been done to reduce the number of needed iterations in Markov chain Monte Carlo. This article focuses on data augmentation, a widely used technique. Due to a large discrepancy between Gibbs step sizes and the rate of posterior concentration in large sample, the posterior samples obtained from existing data augmentations become highly autocorrelated, with the effective sample size too small to be useable. To solve this inefficiency, we propose a family of calibrated data augmentation algorithms, which adjust for this discrepancy by inflating Gibbs step sizes that can vary with the sample size. A Metropolis-Hastings step is included to account for the slight discrepancy between the stationary distribution of the resulting sampler and the exact posterior distribution. Compared to existing alternatives, this approach enjoys much higher effective sample size and much less iterations in sampling. The approach is simple and applicable to a broad variety of existing data augmentation algorithms, and we focus on three popular models: probit, logistic and Poisson log-linear. Dramatic gains in computational efficiency are shown in applications.

KEY WORDS: Bayesian Probit; Bayesian Logit; Big  $n$ ; Data Augmentation; Maximal Correlation; Polya-Gamma for Poisson.

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## 1. Introduction

With the deluge of data in many modern application areas, there is pressing need for scalable computational algorithms for inference from such data, including uncertainty quantification (UQ). Somewhat surprisingly, even as the volume of data increases, uncertainty often remains sizable. Examples in which this phenomenon occurs include financial fraud detection (Ngai et al., 2011), disease mapping (Wakefield, 2007) and online click-through tracking (Wang et al., 2010). Bayesian approaches provide a useful paradigm for quantifying uncertainty in inferences and predictions in these and other settings.

The standard approach to Bayesian posterior computation is Markov chain Monte Carlo (MCMC) and related sampling algorithms. However, it is well known that conventional MCMC algorithms often scale poorly in problem size and complexity. Due to its sequential nature, the computational cost of MCMC is the product of two factors: the evaluation cost at each sampling iteration and the total number of iterations needed to obtain an acceptably low Monte Carlo error. While a substantial literature has developed focusing on decreasing computational cost per iteration (Minsker et al. (2014); Maclaurin and Adams (2014); Srivastava et al. (2015); Conrad et al. (2015) among others), **very little has been done to reduce the needed iterations as the problem size grows.**

**The latter is related to** the properties of the Markov transition kernel; we will refer to this informally as the *mixing properties* of the Markov chain. In the theory literature, many authors have focused on studying mixing properties by showing an ergodicity condition, such as geometric ergodicity (Roberts et al., 2004; Meyn and Tweedie, 2012). This generally yields bounds on the convergence rate and spectral gap of the Markov chain. However, Rajaratnam and Sparks (2015) observe that in many cases, these bounds converge to zero exponentially fast in **ambient dimension  $p$**  or **sample size  $n$** , so that no meaningful guarantee of performance for large problem sizes is provided by most existing bounds.

**The practical consequence is that for some MCMC algorithms under arbitrarily large  $n$  or  $p$ , the Markov chain could completely fail to produce useable posterior samples, regardless how fast each iteration is.** For large  $n$ , Johndrow et al. (2016) discovered that popular data augmentation algorithms, such as the ones for probit (Albert and Chib, 1993) and logistic (Polson et al., 2013) fail to mix the data are imbalanced. An important insight is that the performance can be largely explained by a discrepancy between the rate at which Gibbs step sizes and the width of the high-probability region of the posterior converge to zero as  $n$  increases.

**There has been some related work addressing this mixing issue.** For large  $p$ , in the probability literature, a series of papers have developed an analogue of Harris’ theorem and ergodic theory for infinite-dimensional state spaces (Hairer et al., 2011). Recent work **proposes viable** MCMC algorithms for differential equation models with dimension-independent spectral gap (Hairer et al., 2014). **On the other hand, solution is arguably lacking for large  $n$  problem. As we show in this article, some early ideas to accelerate mixing (Liu and Wu, 1999; Meng and Van Dyk, 1999; Papaspiliopoulos et al., 2007) do not solve the scalability issue even at moderately large  $n$ .**

In this article, we propose a method for increasing Gibbs step sizes by introducing auxiliary parameters that change the variance of full conditional distributions for one or more parameters. **Since the auxiliary parameters can adapt with sample size  $n$ , it fundamentally**

solves the scaling issue of mixing for the involved algorithms. Although we focus on data augmentation algorithms for logit, probit, and Poisson log-linear models, in principle the strategy can be applied more generally to align Gibbs step sizes with the size of the space being explored. As these “calibrated” data augmentation algorithms alter the invariant measure, one can use the Gibbs step as a Metropolis-Hastings proposal, thereby recovering the correct invariant, or view the resulting algorithm as a perturbation of the original Markov chain (Tran et al., 2016). In this article, we focus on the former strategy, showing very substantial practical gains in computational efficiency attributed to our calibration approach. The calibration is simple to obtain for common link functions and generally applicable under more advanced models.

## 2. Calibrated Data Augmentation

Data augmentation Gibbs samplers alternate between sampling latent data  $z$  from their conditional posterior distribution given model parameters  $\theta$  and observed data  $y$ , and sampling parameters  $\theta$  given  $z$  and  $y$ ; either of these steps can be further broken down into a series of full conditional sampling steps but we focus for simplicity on algorithms of the form:

$$\begin{aligned} z &| \theta, y \sim \pi(z; \theta, y) \\ \theta &| z, y \sim f(\theta; z, y), \end{aligned} \tag{1}$$

where  $f$  belongs to a location-scale family, such as the Gaussian. Popular data augmentation algorithms are designed so that both of these sampling steps can be conducted easily and efficiently; e.g., sampling the latent data for each subject independently and then drawing  $\theta$  simultaneously (or at least in blocks) from a multivariate Gaussian or other standard distribution. This effectively avoids the need for tuning, which is a major issue for Metropolis-Hastings algorithms, particularly when  $\theta$  is high-dimensional. Data augmentation algorithms are particularly common for generalized linear models (GLMs), with  $\mathbb{E}(y_i | x_i, \theta) = g^{-1}(x_i \theta)$  and a conditionally Gaussian prior distribution chosen for  $\theta$ . We focus in particular on Poisson log-linear, binomial logistic, and binomial probit as motivating examples.

Consider a Markov kernel  $K((\theta, z); \cdot)$  with invariant measure  $\Pi$  and update rule of the form (1), and a Markov chain  $(\theta_t, z_t)$  on a state space  $\Theta \times \mathcal{Z}$  evolving according to  $K$ . We will abuse notation in writing  $\Pi(d\theta) = \int_{z \in \mathcal{Z}} \Pi(d\theta, dz)$ . The lag-1 autocorrelation for a function  $g : \Theta \rightarrow \mathbb{R}$  at stationarity can be expressed as the Bayesian fraction of missing information (Papaspiliopoulos et al. (2007), Rubin (2004), Liu (1994b))

$$\gamma_g = 1 - \frac{\mathbb{E}[\text{var}(g(\theta) | z)]}{\text{var}(g(\theta))}, \tag{2}$$

where the integrals in the numerator are with respect to  $\Pi(d\theta, dz)$  and in the denominator with respect to  $\Pi(d\theta)$ . Let

$$L_2(\Pi) = \left\{ g : \Theta \rightarrow \mathbb{R}, \int_{\theta \in \Theta} \{g(\theta)\}^2 \Pi(d\theta) < \infty \right\}$$

be the set of real-valued,  $\Pi$  square-integrable functions. The *maximal autocorrelation*

$$\gamma = \sup_{g \in L^2(\Pi)} \gamma_g = 1 - \inf_{g \in L^2(\Pi)} \frac{\mathbb{E}[\text{var}(g(\theta) \mid z)]}{\text{var}(g(\theta))}$$

is equal to the geometric convergence rate of the data augmentation Gibbs sampler (Liu (1994b)). For  $g(\theta) = \theta_j$  a coordinate projection, the numerator of the last term of (2) is, informally, the average squared step size for the augmentation algorithm at stationarity in direction  $j$ , while the denominator is the squared width of the bulk of the posterior in direction  $j$ . Consequently,  $\gamma$  will be close to 1 whenever the average step size at stationarity is small relative to the width of the bulk of the posterior.

The purpose of CDA is to introduce additional parameters that allow us to control the step size relative to the posterior width – roughly speaking, the ratio in (2) – with greater flexibility than reparametrization or parameter expansion. The flexibility gains are achieved by allowing the invariant measure to change as a result of the introduced parameters. The additional parameters, which we denote  $(r, b)$ , correspond to a collection of reparametrizations, each of which defines a proper (but distinct) likelihood  $L_{r,b}(\theta; y)$ , and for which there exists a Gibbs update rule of the form (1). In general,  $b$  will correspond to a location parameter and  $r$  a scale parameter that are tuned to increase  $\mathbb{E}[\text{var}(g(\theta) \mid z)]\{\text{var}(g(\theta))\}^{-1}$ , although the exact way in which they enter the likelihood and corresponding Gibbs update depend on the application. The reparametrization also has the property that  $L_{1,0}(\theta; y) = L(\theta; y)$ , the original likelihood. The resulting Gibbs sampler, which we refer to as CDA Gibbs, has  $\theta$ -marginal invariant measure  $\Pi_{r,b}(\theta; y) \propto L_{r,b}(\theta; y)\Pi^0(\theta)$ , where  $\Pi^0(\theta)$  is the prior. Ultimately, we are interested in  $\Pi_{1,0}(\theta; y)$ , so we use CDA Gibbs as an efficient proposal for Metropolis-Hastings. That is, we propose  $\theta^*$  from  $Q(\theta; \cdot)$  where

$$Q_{r,b}(\theta; A) = \int_{(\theta^*, z) \in A \times \mathcal{Z}} \pi_{r,b}(z; \theta, y) f_{r,b}(\theta^*; z, y) dz d\theta^* \quad (3)$$

for  $A \subseteq \Theta$ , where  $\pi_{r,b}$  and  $f_{r,b}$  denote the conditional densities of  $z$  and  $\theta$  in the Gibbs sampler with invariant measure  $\Pi_{r,b}$ . By tuning working parameters during an adaptation phase to reduce the autocorrelations and increase the Metropolis-Hastings acceptance rate, we can select values of the working parameters that yield a computationally efficient algorithm. Tuning is facilitated by the fact that the M-H acceptance ratios using this proposal kernel have a convenient form, which is a nice feature of using Gibbs to generate M-H proposals.

**Remark 1** *The CDA M-H acceptance ratio is given by*

$$1 \wedge \frac{L(\theta'; y)\Pi^0(\theta')Q_{r,b}(\theta; \theta')}{L(\theta; y)\Pi^0(\theta)Q_{r,b}(\theta'; \theta)} = 1 \wedge \frac{L(\theta'; y)L_{r,b}(\theta; y)}{L(\theta; y)L_{r,b}(\theta'; y)} \quad (4)$$

A general strategy for tuning is given in Section 3.3.

We give a basic convergence guarantee that holds for the CDA M-H under weak assumptions on  $L_{r,b}$ , which is based on (Roberts and Smith, 1994, Theorem 3, also pp. 214). Basically, one needs  $\Pi(\cdot) \ll \Pi_{r,b}(\cdot)$  for all  $r, b$ , where for two probability measures  $\mu, \nu$ ,  $\mu(\cdot) \ll \nu(\cdot)$  means  $\mu$  is absolutely continuous with respect to  $\nu$ .

**Remark 2 (Ergodicity)** Assume that  $\Pi(d\theta)$  and  $\Pi_{r,b}(d\theta)$  have densities with respect to Lebesgue measure on  $\mathbb{R}^p$ , and that  $K_{r,b}((\theta, z); (\theta', z')) > 0 \forall ((\theta, z), (\theta', z')) \in (\Theta \times \mathcal{Z}) \times (\Theta \times \mathcal{Z})$ . Then,

- For fixed  $r, b$ , CDA Gibbs is ergodic with invariant measure  $\Pi_{r,b}(d\theta, dz)$ .
- A Metropolis-Hastings algorithm with proposal kernel  $Q_{r,b}(\theta'; \theta)$  as defined in (3) with fixed  $r, b$  is ergodic with invariant measure  $\Pi(d\theta)$ .

Proofs are located in the Appendix. Remark 2 provides a convergence guarantee, but does not motivate why the convergence properties of CDA are superior to the original Gibbs. Because the algorithms we propose differ in the details of how  $r, b$  enter  $K$ , a general result on convergence rates is not possible. However, we do give several heuristics for why CDA is expected to result in faster convergence in Section 3.

## 2.1 Initial example: probit with intercept only

We use a simple example to illustrate CDA. Consider an intercept-only probit

$$y_i \sim \text{Bernoulli}(p_i), \quad p_i = \Phi(\theta) \quad i = 1, \dots, n$$

and improper prior  $\Pi^0(\theta) \propto 1$ . The basic data augmentation algorithm (Tanner and Wong, 1987; Albert and Chib, 1993) has the update rule

$$z_i \mid \theta, y_i \sim \begin{cases} \text{No}_{[0, \infty)}(\theta, 1) & \text{if } y_i = 1 \\ \text{No}_{(-\infty, 0]}(\theta, 1) & \text{if } y_i = 0 \end{cases} \quad i = 1, \dots, n$$

$$\theta \mid z, y \sim \text{No} \left( n^{-1} \sum_i z_i, n^{-1} \right),$$

where  $\text{No}_{[a,b]}(\mu, \sigma^2)$  is the normal distribution with mean  $\mu$  and variance  $\sigma^2$  truncated to the interval  $[a, b]$ . Johndrow et al. (2016) show that when  $\sum_i y_i = 1$ ,  $\text{var}(\theta_t \mid \theta_{t-1})$  is approximately  $n^{-1} \log n$ , while the width of the high probability region of the posterior is order  $(\log n)^{-1}$ , leading to slow mixing.

As the conditional variance  $\text{var}(\theta \mid z, y)$  is independent of  $z$ , we introduce a scale parameter  $r$  in the update for  $z$ , then adjust the conditional mean by a location parameter  $b$ . This is equivalent to changing the scale of  $z_i \mid \theta, y_i$  from 1 to  $r$  and the mean from  $\theta$  to  $\theta + b$ . These adjustments yield

$$\text{pr}(y_i = 1 \mid \theta, r, b) = \int_0^\infty \frac{1}{\sqrt{2\pi r}} \exp \left( -\frac{(z_i - \theta - b)^2}{2r^2} \right) dz_i = \Phi \left( \frac{\theta + b}{\sqrt{r}} \right), \quad (5)$$

leading to the modified data augmentation algorithm

$$z_i \mid \theta, y_i \sim \begin{cases} \text{No}_{[0, \infty)}(\theta + b, r) & \text{if } y_i = 1 \\ \text{No}_{(-\infty, 0]}(\theta + b, r) & \text{if } y_i = 0 \end{cases} \quad i = 1, \dots, n \quad (6)$$

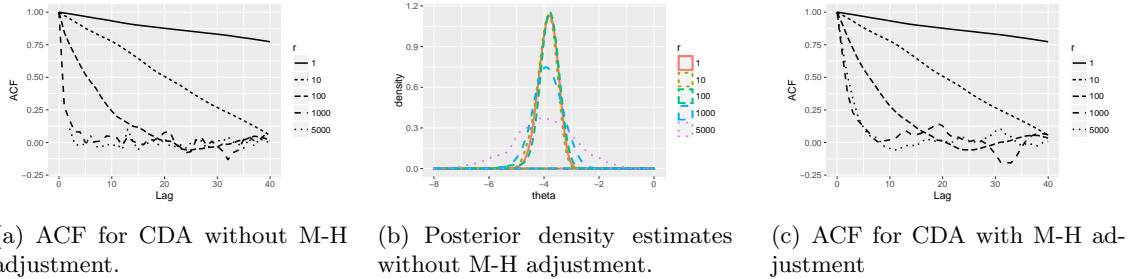
$$\theta \mid z, y \sim \text{No} \left( n^{-1} \sum_i (z_i - b), n^{-1} r \right).$$

To achieve step sizes consistent with the width of the high posterior probability region, we need  $n^{-1}r \approx (\log n)^{-1}$ , so  $r \approx n/\log n$ . To preserve the original target, we use (6) to generate an M-H proposal  $\theta^*$ . By Remark 1, the M-H acceptance probability is given by (4) with  $L_{r,b}(\theta; y_i) = \Phi\left(\frac{\theta+b}{\sqrt{r}}\right)^{y_i} \Phi\left(-\frac{\theta+b}{\sqrt{r}}\right)^{(1-y_i)}$  and  $L(\theta; y_i) = L_{1,0}(\theta; y_i)$ . Setting  $r_i = 1$  and  $b_i = 0$  leads to acceptance rate of 1, which corresponds to the original Gibbs sampler.

To illustrate, we consider  $\sum_i y_i = 1$  and  $n = 10^4$ . Letting  $r = n/\log n$ , we then choose the  $b_i$ 's to increase the acceptance rate in the M-H step. In this simple example, it is easy to compute a “good” value of  $b_i$ , since  $b_i = -3.7(\sqrt{r} - 1)$  results in  $\text{pr}(y_i = 1) = \Phi(-3.7) = n^{-1} \sum_i y_i \approx 10^{-4}$  in the proposal distribution, centering the proposals near the MLE for  $p_i$ .

We perform computation for these data with different values of  $r$  ranging from  $r = 1$  to  $r = 5,000$ , with  $r = 1,000 \approx n/\log n$  corresponding to the theoretically optimal value. Figure 2(a) plots autocorrelation functions (ACFs) for these different samplers without M-H adjustment. Autocorrelation is very high even at lag 40 for  $r = 1$ , while increasing  $r$  leads to dramatic improvements in mixing. There are no further gains in increasing  $r$  from the theoretically optimal value of  $r = 1,000$  to  $r = 5,000$ . Figure 2(b) shows kernel-smoothed density estimates of the posterior of  $\theta$  without M-H adjustment for different values of  $r$  and based on long chains to minimize the impact of Monte Carlo error; the posteriors are all centered on the same values but with variance increasing somewhat with  $r$ . With M-H adjustment such differences are removed; the M-H step has acceptance probability close to one for  $r = 10$  and  $r = 100$ , about 0.6 for  $r = 1,000$ , and 0.2 for  $r = 5,000$ . The autocorrelation functions for CDA M-H in this case are very similar to those for CDA Gibbs (compare Figure 2(a) to Figure 2(c)), indicating that it is possible to retain the good convergence properties of CDA Gibbs in a Markov chain with the target invariant measure.

Figure 1: Autocorrelation functions (ACFs) and kernel-smoothed density estimates for different CDA samplers in intercept-only probit model.



### 3. Specific algorithms

In this section, we describe CDA algorithms for general probit and logistic regression, and describe a general strategy for tuning  $r, b$ .

### 3.1 Probit regression

We now generalize to a probit regression:

$$y_i \sim \text{Bernoulli}(p_i), \quad p_i = \Phi(x_i\theta) \quad i = 1, \dots, n$$

with improper prior  $\Pi^0(\theta) \propto 1$ . The data augmentation sampler Tanner and Wong (1987); Albert and Chib (1993) has the update rule

$$z_i \mid \theta, x_i, y_i \sim \begin{cases} \text{No}_{[0, \infty)}(x_i\theta, 1) & \text{if } y_i = 1 \\ \text{No}_{(-\infty, 0]}(x_i\theta, 1) & \text{if } y_i = 0 \end{cases} \quad i = 1, \dots, n$$

$$\theta \mid z, x, y \sim \text{No}((X'X)^{-1}X'z, (X'X)^{-1}).$$

Liu and Wu (1999) and Meng and Van Dyk (1999), among others, previously studied this algorithm and proposed to rescale  $\theta$  through parameter expansion. However, this modification does not impact the conditional variance of  $\theta$  and thus does not directly increase typical step sizes.

Our approach is fundamentally different, since we directly adjust the conditional variance. Similar to the intercept only model, we modify  $\text{var}(\theta|z)$  by changing the scale of each  $z_i$ . Since the conditional variance is now a matrix, for flexible tuning, we let  $r$  and  $b$  vary over index  $i$ , yielding update rule

$$z_i \mid \theta, x_i, y_i \sim \begin{cases} \text{No}_{[0, \infty)}(x_i\theta + b_i, r_i) & \text{if } y_i = 1 \\ \text{No}_{(-\infty, 0]}(x_i\theta + b_i, r_i) & \text{if } y_i = 0 \end{cases} \quad i = 1, \dots, n \quad (7)$$

$$\theta \mid z, X \sim \text{No}((X'R^{-1}X)^{-1}X'R^{-1}(z - b), (X'R^{-1}X)^{-1}),$$

where  $R = \text{diag}(r_1, \dots, r_n)$ ,  $b = (b_1, \dots, b_n)'$ , under the Bernoulli likelihood:

$$\text{pr}(y_i = 1 \mid \theta, x_i, r_i, b_i) = \int_0^\infty \frac{1}{\sqrt{2\pi r_i}} \exp\left(-\frac{(z_i - x_i\theta - b_i)^2}{2r_i}\right) dz_i = \Phi\left(\frac{x_i\theta + b_i}{\sqrt{r_i}}\right). \quad (8)$$

For fixed  $r = (r_1, \dots, r_n)$  and  $b = (b_1, \dots, b_n)$ , (8) defines a proper Bernoulli likelihood for  $y_i$  conditional on parameters, and therefore the transition kernel  $K_{r,b}((\theta, z); \cdot)$  defined by the Gibbs update rule in (7) would have a unique invariant measure for fixed  $r, b$ , which we denote  $\Pi_{r,b}(\theta, z \mid y)$ . (8) suggests that another way to view CDA Gibbs is that a different link function is chosen for each observation, and the corresponding M-H algorithm allows us to recover the posterior under the original link. The CDA M-H algorithm in this case proposes from  $Q(\theta^*; \theta) = \int f(\theta^*; z, y)\pi(z; \theta, y)dz$ , the  $\theta$ -marginal of the transition kernel  $K_{r,b}((\theta^*, z^*); (\theta, z))$ . The acceptance probability is given by (4) with  $L_{r,b}(\eta_i; y_i) = \Phi\left(\frac{\eta_i + b}{\sqrt{r}}\right)^{y_i} \Phi\left(-\frac{\eta_i + b}{\sqrt{r}}\right)^{(1-y_i)}$ ; we denote  $L_{1,0}$  by  $L$ .

For insight into the relationship between  $r$  and step size, consider the  $\theta$ -marginal autocovariance in a Gibbs sampler evolving according to  $K_{r,b}$ :

$$\begin{aligned} \text{cov}_{r,b}(\theta_t \mid \theta_{t-1}, X, z, y) &= (X'R^{-1}X)^{-1} + (X'R^{-1}X)^{-1}X'R^{-1}\text{cov}(z - b \mid R)R^{-1}X(X'R^{-1}X)^{-1} \\ &\geq (X'R^{-1}X)^{-1}, \end{aligned} \quad (9)$$

In the special case where  $r_i = r_0$  for all  $i$ , we have

$$\text{cov}_{r,b}(\theta_t \mid \theta_{t-1}, X, z, y) \geq r_0(X'X)^{-1},$$

so that all of the conditional variances are increased by at least a factor of  $r_0$ . This holds uniformly over the entire state space, so it follows that

$$\mathbb{E}_{\Pi_{r,b}}[\text{var}(\theta_j | z)] \geq r_0 \mathbb{E}_{\Pi}[\text{var}(\theta_j | z)].$$

Of course, this auxiliary Gibbs step is used to generate proposals, so the key to CDA is to choose  $r, b$  to make  $\mathbb{E}_{\Pi_{r,b}}[\text{var}(\theta_j | z)]$  close to  $\text{var}_{\Pi_{r,b}}(\theta_j | z)$ , while additionally maximizing the M-H acceptance probability. We defer the choice for  $r, b$  and their effects to the last subsection.

### 3.2 Logistic regression

Calibration was easy to achieve in the probit examples, because  $\text{var}(\theta|z, y)$  does not involve the latent variable  $z$ . In cases in which the latent variable impacts the variance of the conditional posterior distribution of  $\theta$ , we propose to stochastically increase  $\text{var}(\theta|z, y)$  by modifying the distribution of  $z$ . We focus on the logistic regression model with

$$y_i \sim \text{Bernoulli}(p_i), \quad p_i = \frac{\exp(x_i \theta)}{1 + \exp(x_i \theta)} \quad i = 1, \dots, n$$

and improper prior  $\Pi^0(\theta) \propto 1$ . For this model, Polson et al. (2013) proposed Polya-Gamma data augmentation:

$$\begin{aligned} z_i &\sim \text{PG}(1, |x_i \theta|) \quad i = 1, \dots, n, \\ \theta &\sim \text{No}((X'ZX)^{-1}X'(y - 0.5), (X'ZX)^{-1}), \end{aligned}$$

where  $Z = \text{diag}(z_1, \dots, z_n)$ . This algorithm relies on expressing the logistic regression likelihood as

$$L(x_i \theta; y_i) = \int \exp\{x_i \theta (y_i - 1/2)\} \exp\left\{-\frac{z_i (x_i \theta)^2}{2}\right\} \text{PG}(z_i | 1, 0) dz_i,$$

where  $\text{PG}(a_1, a_2)$  denotes the Polya-Gamma distribution with parameters  $a_1, a_2$ , with  $\mathbb{E}z_i = \frac{a_1}{2a_2} \tanh(\frac{a_2}{2})$ .

We replace  $\text{PG}(z_i | 1, 0)$  with  $\text{PG}(z_i | r_i, 0)$  in the step for updating the latent data. Since  $\mathbb{E}_z \text{var}(\theta|z, y)$  lacks closed-form, we focus on the precision matrix  $\mathbb{E}_z(\text{var}(\theta|z, y))^{-1} = X' \mathbb{E} Z X$ . Smaller  $r_i$  can lead to smaller  $\mathbb{E}z_i$ , providing a route to calibration. Applying the bias-adjustment term  $b_i$  to the linear predictor  $\eta_i = x_i \theta$  leads to

$$\begin{aligned} L_{r,b}(x_i \theta; y_i) &= \int_0^\infty \exp\{(x_i \theta + b_i)(y_i - r_i/2)\} \exp\left\{-\frac{z_i (x_i \theta + b_i)^2}{2}\right\} \text{PG}(z_i | r_i, 0) dz_i \\ &= \frac{\exp\{(x_i \theta + b_i)y_i\}}{\{1 + \exp(x_i \theta + b_i)\}^{r_i}}, \end{aligned} \tag{10}$$

and the update rule for the proposal (also the CDA Gibbs sampler)

$$\begin{aligned} z_i &\sim \text{PG}(r_i, |x_i \theta + b_i|) \quad i = 1, \dots, n, \\ \theta^* &\sim \text{No}((X'ZX)^{-1}X'(y - r/2 - Zb), (X'ZX)^{-1}), \end{aligned}$$

where  $r = (r_1, \dots, r_n)$ . By (4), the M-H acceptance probability is

$$1 \wedge \prod_i \frac{\{1 + \exp(x_i \theta)\} \{1 + \exp(x_i \theta^* + b_i)\}^{r_i}}{\{1 + \exp(x_i \theta^*)\} \{1 + \exp(x_i \theta + b_i)\}^{r_i}}.$$



### 3.3 Choice of calibration parameters

As illustrated in the previous subsection, efficiency of CDA is dependent on a good choice of the calibration parameters  $r = (r_1, \dots, r_n)$  and  $b = (b_1, \dots, b_n)$ . In the intercept-only case for probit, it was possible to analytically calculate appropriate values of these parameters, but in general an empirical approach is needed. We now propose a simple and efficient algorithm for calculating “good” values of these parameters relying on Fisher information.

In large samples, the inverse of Fisher information evaluated at the posterior mode is a useful approximation to the posterior covariance. **Our goal is to adjust the conditional variance under calibration of  $(r, b)$ , to approximately match the marginal variance under the exact target distribution.** Therefore, depending on which one is more convenient to compute, it is useful to choose  $(r, b)$  to minimize one of the distances:

$$\begin{aligned}\Delta_{\mathcal{I}}(\hat{\theta}_{MAP}) &= \text{dist} \left[ \mathcal{I}_{y|\theta}(\theta), \mathbb{E}_{z|\theta} \mathcal{I}_{y|\theta,z}(\theta; r, b) \right] \Big|_{\hat{\theta}_{MAP}} \\ \Delta_{\mathcal{I}^{-1}}(\hat{\theta}_{MAP}) &= \text{dist} \left[ \mathcal{I}_{y|\theta}^{-1}(\theta), \mathbb{E}_{z|\theta} \mathcal{I}_{y|\theta,z}^{-1}(\theta; r, b) \right] \Big|_{\hat{\theta}_{MAP}}\end{aligned}$$

where  $\text{dist}(A, B)$  denotes a metric such as Euclidean distance  $\|A - B\|_2$  or Rao’s distance  $\{\text{tr}[\log(A^{-1/2}BA^{-1/2})^2]\}^{1/2}$  with  $\text{tr}$  as the trace (Atkinson and Mitchell, 1981);  $\mathbb{E}_{z|\theta}$  is taken over the conditional distribution of  $z$  under  $L_{r,b}(\theta; y)$ ;  $\hat{\theta}_{MAP}$  is the posterior mode under the target likelihood-prior product  $L(y; \theta)\Pi^0(\theta)$ . The two matrices consist of elements

$$\begin{aligned}(\mathcal{I}_{y|\theta}(\theta))_{i,j} &= \mathbb{E}_{y|\theta} \left[ \left( \frac{\partial}{\partial \theta_i} \log L(y; \theta) \right) \left( \frac{\partial}{\partial \theta_j} \log L(y; \theta) \right) \right], \\ (\mathcal{I}_{y|\theta,z}(\theta; r, b))_{i,j} &= \mathbb{E}_{y|\theta,z} \left[ \left( \frac{\partial}{\partial \theta_i} \log L_{r,b}(y, z; \theta) \right) \left( \frac{\partial}{\partial \theta_j} \log L_{r,b}(y, z; \theta) \right) \right]\end{aligned}$$

for  $i = 1, \dots, p$ ,  $j = 1, \dots, p$ , with  $\mathbb{E}_{y|\theta}$  taken over the distribution of  $y$  under the target marginal  $L(y; \theta)$  and  $\mathbb{E}_{y|\theta,z}$  taken over conditional distribution of  $y$  under the augmented  $L_{r,b}(y, z; \theta)$  with the calibration of  $(r, b)$ . These inverses of these two matrices are approximations to  $\text{var}(\theta | y)$  and  $\text{var}(\theta | z, y)$ . Moreover, if  $L_{r,b}(y, z; \theta)$  has  $\theta$  following a Gaussian, we would have  $\mathcal{I}_{y|\theta,z}^{-1}(\theta) = \text{var}(\theta | z, y)$  exactly.

Computing full Fisher information may appear challenging and problem-specific, however, there often exists a simple and common solution of  $(r, b)$  for each class of data augmentation. Different models using the same type of data augmentation usually share a common form of conditional likelihood, given their own mapping of  $\eta(\theta) : \mathbb{R}^p \rightarrow \mathbb{R}^d$ . For example, a class of models under Bernoulli probit link share common form  $y_i | \eta_i(\theta) \stackrel{iid}{\sim} \text{Bernoulli}(\Phi(\eta_i(\theta)))$ , even though  $\eta_i(\theta)$  may have unique dependent structure over  $i$  in different models (e.g.  $\eta_i(\theta) = x_i\theta$  or  $\eta_i(\theta) = \theta_i$ ). Exploiting this common form, one can calibrate based on the Fisher information of  $\eta$  for this whole class of models, instead of  $\theta$  for each model. Using simple chain rule, observe

$$\begin{aligned}\mathcal{I}_{y|\theta}(\theta) &= \dot{\eta} \mathcal{I}_{y|\eta}(\eta(\theta)) \dot{\eta}', \\ \mathcal{I}_{y|\theta,z}(\theta; r, b) &= \dot{\eta} \mathcal{I}_{y|\eta,z}(\eta(\theta); r, b) \dot{\eta}'\end{aligned}$$

where  $\dot{\eta}$  denotes the  $p$ -by- $d$  gradient matrix consisting of the partial derivative  $\frac{\partial \eta_k(\theta)}{\partial \theta_j}$  of the  $k$ th output  $\eta_k(\theta)$  with respect to  $\theta_j$ . Although  $\dot{\eta}$  vary across different models, it is the same in two Fisher information matrices. Therefore, one only need to reduce the difference between  $\mathcal{I}_{y|\theta}(\eta(\theta))$  and  $\mathcal{I}_{y|\theta,z}(\eta(\theta); r, b)$ , without having to compute the full Fisher information based on  $\theta$ . In all algorithms presented in this article,  $\mathcal{I}_{y|\theta}(\eta(\theta))$  and  $\mathcal{I}_{y|\theta,z}(\eta(\theta); r, b)$  are simple diagonal matrices, and it can be made exactly  $I_{y|\theta}(h(\theta)) = I_{y|\theta,z}(\theta; r, b)$ , leading to  $\Delta_{\mathcal{I}}(\theta) = 0$  or  $\Delta_{\mathcal{I}^{-1}}(\theta) = 0$  for given  $\theta$ .

In general, since we do not have access to the posterior mode, we instead use samples from the Markov chain during an adaptation phase to dynamically update  $r_t, b_t$ . Specifically, we choose  $r_{t+1}$  to minimize  $\Delta_{\mathcal{I}}(\theta_t)$  or  $\Delta_{\mathcal{I}^{-1}}(\theta_t)$ , and set  $b_{t+1}$  to minimize the difference between  $L_{1,0}(\theta_t; y)$  and  $L_{r_{t+1}, b_{t+1}}(\theta_t; y)$ . Thus, we use  $r$  to adjust the conditional variance based on  $L_{r,b}$  to match the marginal variance based on  $L$  and  $b$  to make  $L_{r,b}$  close to  $L_{1,0}$  in the neighborhood of  $\theta_t$ . Intuitively, this will make the target distribution closer to the invariant measure of calibrated Gibbs, and correspondingly increase the MH acceptance rate. **Some illustrative results about the adaptation is provided in the appendix.**

The proposal kernel we describe above is *adaptive*; that is, we have a collection of proposal kernels  $\mathcal{Q} = \{Q_{r,b}\}_{(r,b) \in \mathbb{R}_+ \times \mathbb{R}}$ , and we choose a different member of  $\mathcal{Q}$  at each iteration to create the proposal. The *target* for the resulting transition kernel is  $\Pi_{1,0}$  for every  $Q_{r,b}$  because of the Metropolis-Hastings rejection step. In general, ergodicity of adaptive algorithms requires a diminishing adaptation condition; a general condition of this sort is given in Roberts and Rosenthal (2007). Although the algorithm we describe is unlikely to satisfy diminishing adaptation if updating of  $r, b$  continues indefinitely, the condition is trivially satisfied by any algorithm that stops adaptation after a fixed number of iterations. Thus, for simplicity, we choose a tuning period length, after which we fix  $r, b$  at their current values. More sophisticated adaptation schemes could be devised; however, the fixed tuning period works well empirically.

For a concrete illustration, we first return to the first example of probit regression. Putting  $\eta_i = x_i \theta$ , we obtain

$$\mathcal{I}_{y|\theta}(\theta) = X' \text{diag} \left\{ \frac{\phi(\eta_i)^2}{\Phi(\eta_i)(1 - \Phi(\eta_i))} \right\} X, \quad \mathbb{E}_{z|\theta} \mathcal{I}_{y|\theta,z}(\theta; r, b) = X' R^{-1} X$$

where  $\phi$  is the standard normal density. **Setting  $\Delta_{\mathcal{I}}(\theta_t) = 0$  and  $L_{r,b}(\eta_i; y_i) = L(\eta_i; y_i)$  to locally increase the acceptance rate in the M-H step, this yields tuning solution for Bernoulli probit regression**

$$r_i = \frac{\Phi(\eta_i)(1 - \Phi(\eta_i))}{\phi(\eta_i)^2},$$

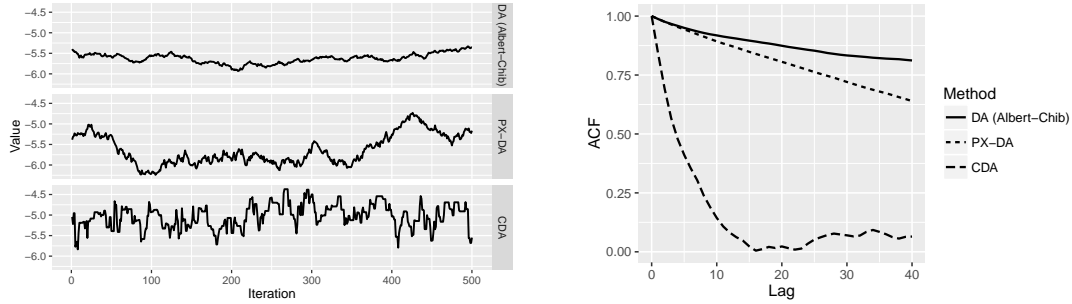
$$b_i = \eta_i(\sqrt{r_i} - 1).$$

**Note  $X'$  is a special case of the gradient  $\dot{\eta}$  when  $\eta_i = x_i \theta$ . For Bernoulli probit model with other forms of  $\eta_i$ , the solution for tuning parameters stay the same.**

To illustrate, we consider a probit regression with an intercept and two predictors  $x_{i,1}, x_{i,2} \sim \text{No}(1, 1)$ , with  $\theta = (-5, 1, -1)'$ , generating  $\sum y_i = 20$  among  $n = 10,000$ . The Albert and Chib (1993) DA algorithm mixes slowly (Figure 3(a) and 3(b)). We also show the results of the parameter expansion algorithm (PX-DA) proposed by Liu and Wu

(1999). PX-DA only mildly reduces the correlation, as it does not solve the small step size problem. For CDA, we tuned  $r$  and  $b$  for 100 steps using the Fisher information, reaching a satisfactory acceptance rate of 0.6. Applying CDA afterwards, we obtain dramatically better mixing.

Figure 2: Panel (a) demonstrates in traceplot and panel (b) in autocorrelation the substantial improvement in CDA by correcting the variance mis-match in probit regression with rare event data, compared with the original (Albert and Chib, 1993) and parameter-expanded methods (Liu and Wu, 1999).



(a) Traceplot for the original DA, parameter expanded DA and CDA algorithms.

(b) ACF for original DA, parameter expanded DA and CDA algorithms.

For the second example of logistic regression, taking  $\eta_i = x_i\theta$ , the Fisher information matrices are:

$$\begin{aligned}\mathcal{I}_{y|\theta}(\theta) &= X' \text{diag} \left\{ \frac{\exp(\eta_i)}{\{1 + \exp(\eta_i)\}^2} \right\} X, \\ \mathbb{E}_{z|\theta} \mathcal{I}_{y|\theta, z}(\theta; r, b) &= X' \text{diag} \left\{ \frac{r_i}{2|\eta_i + b_i|} \tanh \left( \frac{|\eta_i + b_i|}{2} \right) \right\} X.\end{aligned}$$

Setting  $\Delta_{\mathcal{I}}(\theta_t) = 0$  and  $\{1 + \exp(\eta_i)\} = \{1 + \exp(\eta_i + b_i)\}^{r_i}$  to locally maximize the M-H acceptance rate yields

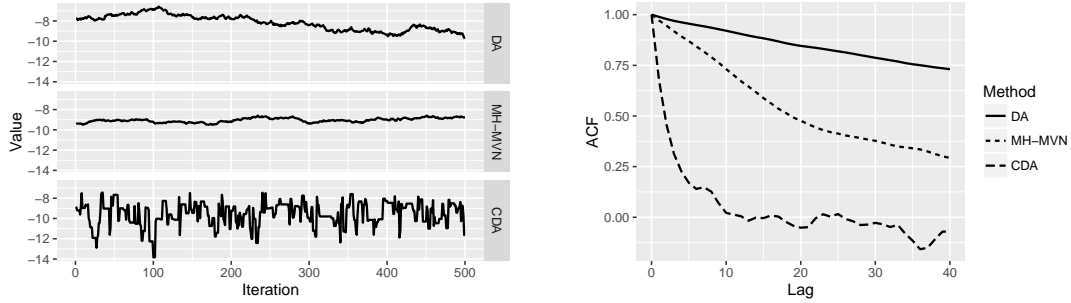
$$\begin{aligned}r_i &= \frac{\exp(\eta_i)}{\{1 + \exp(\eta_i)\}^2} 2|\eta_i + b_i| / \tanh \left( \frac{|\eta_i + b_i|}{2} \right), \\ b_i &= \log[\{1 + \exp(\eta_i)\}^{1/r_i} - 1] - \eta_i.\end{aligned}$$

Again, this tuning solution is invariant to the different forms of  $\eta$  under the Bernoulli logistic model.

To illustrate, we use a two parameter intercept-slope model with  $x_1 \sim \text{No}(0, 1)$  and  $\theta = (-9, 1)'$ . With  $n = 10^5$ , we obtain rare outcome data with  $\sum y_i = 50$ . Besides the original DA algorithm (Polson et al., 2013), we also consider an M-H sampler using a multivariate normal proposal  $\theta^*|\theta \sim \text{No}(\theta^*|\theta, \mathcal{I}^{-1}(\theta))$  with the inverse Fisher information as the covariance. Similarly, we test an alternative of using DA to generate new  $\theta^*$ , and scaling to  $\theta^{**} = \theta + \alpha(\theta^* - \theta)$  with  $\alpha \geq 1$  as an M-H proposal. Both M-H with a normal

proposal and with scaled proposal suffer from low acceptance rate, unless  $\alpha \approx 1$  in the latter (corresponding to almost no adjustment from DA). For CDA we tuned  $r$  and  $b$  for 100 steps using the Fisher information, reaching an acceptance rate of 0.8. Shown in Figure 3, DA and simple M-H mix slowly, exhibiting strong autocorrelation even at lag 40, while CDA has dramatically better mixing.

Figure 3: Panel (a) demonstrates in traceplot and panel (b) in autocorrelation the substantial improvement of CDA in logistic regression with rare event data, compared with the original DA (Polson et al., 2013) and the M-H algorithm with multivariate normal proposal (MH-MVN).



(a) Traceplots for DA, CDA and M-H with multivariate normal proposal.

(b) ACF for DA, CDA and M-H with multivariate normal proposal.

#### 4. Simulation Study: Scaling to Massive $n$

As motivated above, two factors are necessary for obtaining useable posterior samples within a practical time: a low computing cost in each iteration and a high effective sample size within small number of iterations. We first demonstrate that calibration can solve the scalability issue in the latter.

To start, we consider a simple Bernoulli logistic regression with a common intercept:

$$y_i \stackrel{iid}{\sim} \text{Bernoulli}\left(\frac{\exp(\theta)}{1 + \exp(\theta)}\right), \quad i = 1, \dots, n,$$

with flat improper prior for  $\theta$ . As the likelihood is  $L(y; \theta) = \frac{\exp(\theta \sum y_i)}{(1 + \exp(\theta))^n}$ , it enjoys efficient computing per iteration that only involves 1 Polya-Gamma latent variable. Using calibration parameters  $(r, b)$ , new proposal can be simulated from

$$\begin{aligned} z &\sim \text{PG}(nr, \theta + b) \\ \theta^* &\sim \text{No}\left(\frac{\sum y_i - rn/2 - zb}{z}, \frac{1}{z}\right), \end{aligned}$$

and M-H acceptance step as described above using  $L_{r,b}(\theta; y) = \frac{\exp(\theta+b)\sum y_i}{\{1+\exp(\theta+b)\}^{nr}}$ . To have a proper  $L_{r,b}(\theta; y)$ , we further require  $r \geq (\sum y_i - 1)/n + \epsilon$  with  $\epsilon$  a small positive constant. As usual, one would obtain the Gibbs sampling algorithm (Polson et al., 2013) via  $(r, b) = (1, 0)$ . Using Fisher information, the parameters are adapted initially for 200 steps, via  $r = \frac{\exp(\theta)}{\{1+\exp(\theta)\}^2} / \left( \frac{1}{2|\theta+b|} \tanh \frac{|\theta+b|}{2} \right) \vee ((\sum y_i - 1)/n + \epsilon)$  and  $b = \log[\{1 + \exp(\theta)\}^{1/r} - 1] - \theta$ .

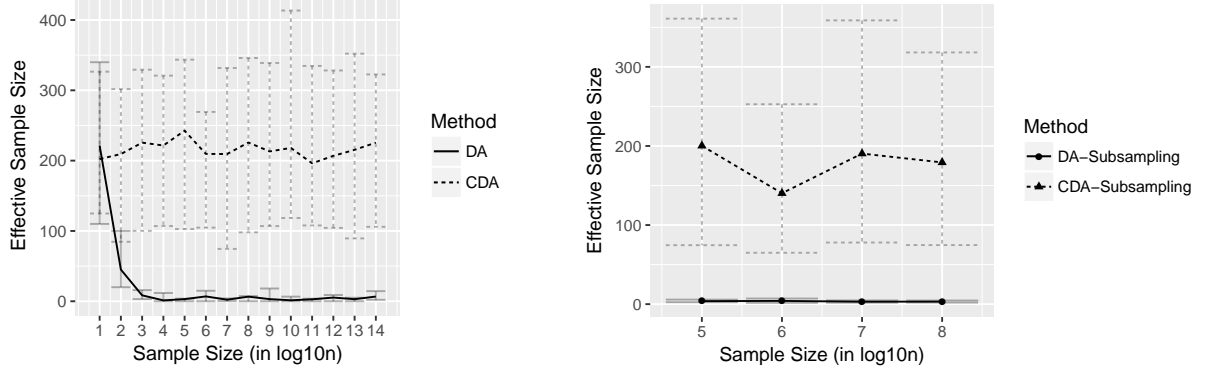
To mimic the large variance discrepancy that grows with  $n$ , we fixed  $\sum y_i = 1$  and increase  $n$  from  $10^1$  to a massive  $10^{14}$ . Figure 4(a) compares the effective sample size per 1,000 steps using DA and CDA. Surprisingly, the deterioration of DA shows as early as  $n = 10^2$  in comparison; its slow-down becomes critical at  $n = 10^4$  with effective sample size close to 0. CDA performs exceptionally well, even at massive  $n = 10^{14}$  (we stop at  $10^{14}$  as  $1/n$  reaches the limit of floating point accuracy).

In more complicated settings, one issue for data augmentation in general is the large number of latent variables to sample in each iteration. The common strategy is to utilize random sub-sample of data at much smaller size and build approximating algorithm (Quiroz et al., 2016; Johndrow et al., 2017). Although this is not the focus of this article, we show that it does not solve the scalability issue by only accelerating the computation within one iteration. Instead, one can couple CDA with these algorithms to obtain efficient posterior sample within a short time.

We consider the same two-parameter intercept-slope model in logistic regression as described in the last section, except we now vary sample size from  $n = 10^5$  to  $10^8$ . We simulate Bernoulli outcome  $y_i \sim \text{Bernoulli}(\frac{1}{1+\exp(-x_i\theta)})$  based on  $x_1 \sim \text{No}(0, 1)$  and  $\theta = (-\theta_0, 1)'$ . We vary  $\theta_0$  and induce  $\sum y_i \approx 10$  for each  $n$ . We utilize the sub-sampled-Polya-Gamma algorithm described by Johndrow et al. (2017), and apply CDA to calibrate the variance discrepancy. Since  $y$  is highly imbalanced in the number of 0 and 1, we apply biased-sampling by including all data with  $y_i = 1$ , while sub-sampling 1% of data with  $y_i = 0$ . The algorithmic details and the calibrated form are presented in the appendix.

Figure 4(b) compares the performance of the two approximating algorithms, one combining CDA and sub-sampling, and one that using sub-sampling alone. Clearly, only accelerating each step via sub-sampling does not solve the inefficiency with very low effective sample size; while using CDA and sub-sampling together can produce fast mixing sample within a reasonable time.

Figure 4: CDA can maintains high effective sample size, even when scaling to massive  $n$ . Panel(a) shows the performance of DA and CDA when  $n$  is scaled up to  $10^{14}$ ; Panel(b) shows the performance of CDA and DA, coupled with sub-sampling approximation to reduce the number of sampled latent variables. Only accelerating computing time in each iteration (DA-Subsampling) does not solve the scalability issue in low effective sample size.



(a) Effective sample size per 1,000 steps with different sample size  $n$  from  $10$  to  $10^{14}$ , using logistic regression model with intercept only.

(b) Effective sample size per 1,000 steps with different  $n$  from  $10^5$  to  $10^8$ , in logistic regression with slope and intercept, using sub-sampling.

## 5. Co-Browsing Behavior Application

We apply CDA to an online browsing activity dataset. The dataset contains a two-way table of visit count by users who browsed one of 96 client websites of interest, and one of the  $n = 59,792$  high-traffic sites during the same browsing session. We refer to visiting more than one site during the same session as co-browsing. For each of the client websites, it is of large commercial interest to find out the high-traffic sites with relatively high co-browsing rates, so that ads can be more effectively placed. For the computational advertising company, it is also useful to understand the co-browsing behavior and predict the traffic pattern of users. We consider two models for these data.

### 5.1 Hierarchical Binomial Model for Co-Browsing Rates

We initially focus on one client website and analyze co-browsing rates with the high-traffic sites. With the total visit count  $N_i$  available for the  $i$ th high-traffic site, the count of co-browsing  $y_i$  can be considered as the result of a binomial trial. With  $y_i$  extremely small relative to  $N_i$  (ratio  $0.00011 \pm 0.00093$ ), the maximum likelihood estimate  $y_i/N_i$  can have poor performance. For example, when  $y_i = 0$ , estimating the rate as exactly 0 is not ideal. Therefore, it is useful to consider a hierarchical model to allow borrowing of information across high-traffic sites:

$$y_i \sim \text{Binomial} \left( N_i, \frac{\exp(\theta_i)}{1 + \exp(\theta_i)} \right), \quad \theta_i \stackrel{iid}{\sim} \text{No}(\theta_0, \sigma_0^2), \quad i = 1 \dots n$$

$$(\theta_0, \sigma_0^2) \sim \pi(\theta_0, \sigma_0^2)$$

Based on expert opinion in quantitative advertising, we use a weakly informative prior  $\theta_0 \sim \text{No}(-12, 49)$  and uniform prior on  $\sigma_0^2$ . Similar to the logistic regression, we calibrate the binomial Polya-Gamma augmentation, leading to the proposal likelihood:

$$L_{r,b}(\theta_i; y_i, N_i, r_i, b_i) = \frac{\exp(\theta_i + b_i)_i^y}{\{1 + \exp(\theta_i + b_i)\}^{N_i r_i}}$$

Conditioned on the latent Polya-Gamma latent variable  $z_i$ , each proposal  $\theta_i^*$  can be sampled from:

$$z_i \sim \text{PG}((N_i r_i), \theta_i + b_i) \\ \theta_i^* \sim \text{No}\left(\frac{y_i - r_i N_i / 2 - z_i b_i + \theta_0 / \sigma_0^2}{z_i + 1 / \sigma_0^2}, \frac{1}{z_i + 1 / \sigma_0^2}\right),$$

and accepted or rejected using an M-H step. We further require  $r_i \geq (y_i - 1)/N_i + \epsilon$  to have a proper  $L_{r,b}(\theta_i; y_i, N_i)$  with  $\epsilon$  a small constant. Similar to logistic regression, the auxiliary parameters are chosen as  $r_i = \frac{\exp(\theta_i)}{\{1 + \exp(\theta_i)\}^2} / \left( \frac{1}{2|\theta_i + b_i|} \tanh \frac{|\theta_i + b_i|}{2} \right) \vee ((y_i - 1)/N_i + \epsilon)$  and  $b_i = \log[\{1 + \exp(\theta_i)\}^{1/r_i} - 1] - \theta_i$  during adaptation. Since  $\theta_i$ 's are conditionally independent, the calibrated proposal can be individually accepted with high probability for each  $i$ . This leads to a high average acceptance of 0.9, despite the high dimensionality of 59,792  $\theta_i$ 's. After  $\theta_i$ 's are updated, other parameters are sampled from

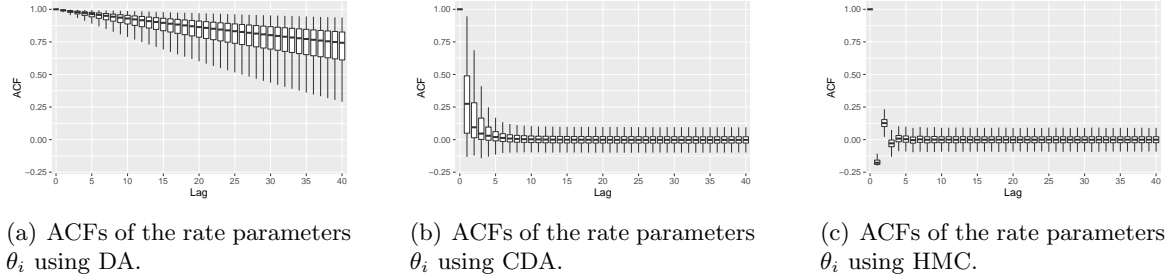
$$\theta_0 \sim \text{No}\left((n/\sigma^2 + 1/49)^{-1} \left( \sum_i \theta_i / \sigma^2 - 12/49 \right), (n/\sigma^2 + 1/49)^{-1}\right),$$

and  $\sigma_0^2 \sim \text{Inverse-Gamma}(n/2 - 1, \sum_i (\theta_i - \theta_0)^2 / 2)$ .

Figure 5 shows the boxplots of the ACFs for all  $\theta_i$ 's. We compare the result with the original DA (Polson et al., 2013) and Hamiltonian Monte Carlo (HMC) provided by the STAN software (Carpenter et al., 2016). We run DA for 100,000 steps, HMC for 2,000 steps and CDA for 2,000 steps, so that they have approximately the same effective sample size (calculated with the CODA package in R). All of the parameters mix poorly in DA; HMC and CDA lead to significant improvement with autocorrelation rapidly decaying to close to zero within 5 lags.

Shown in Table 1, CDA and HMC have very close estimates in posterior means and 95% credible intervals for the parameters, while DA has poor estimates due to critically slow mixing. The difference between HMC and CDA is that, although HMC is slightly more efficient in effective sample size per iteration ( $T_{eff}/T$ ) for this model, it is much more computationally intensive and generates many fewer iterations than CDA within the same budget of computing time. As the result, CDA has the most efficient computing time per effective sample.

Figure 5: Boxplots of the ACFs show the mixing of the 59,792 parameters in the hierarchical binomial model, for the original DA(Polson et al., 2013), CDA and HMC.



	DA	CDA	HMC
$\sum \theta_i/n$	-10.03 (-10.16, -9.87)	-12.05 (-12.09, -12.02)	-12.06 (-12.09, -12.01)
$\sum \theta_i^2/n$	102.25 (98.92, 105.23)	153.04 (152.06, 154.05)	153.17 (152.02, 154.29)
$\theta_0$	-10.03 (-10.17, -9.87)	-12.05 (-12.09, -12.01)	-12.06 (-12.10, -12.01)
$\sigma^2$	1.60 (1.36, 1.82)	7.70 (7.49, 7.88)	7.71 (7.51, 7.91)
$T_{eff}/T$	0.0085 (0.0013, 0.0188)	0.5013 (0.1101, 1.0084)	0.8404 (0.5149, 1.2470)
Avg Computing Time / $T$	1.2 sec	1.2 sec	6 sec
Avg Computing Time / $T_{eff}$	140.4 sec	0.48 sec	1.3 sec

Table 1: Parameter estimates (with 95% credible intervals) and computing speed (ratios among computing time, effective sample sizes  $T_{eff}$  and total iterations  $T$ ) of the DA, CDA and HMC in hierarchical binomial model. CDA provides parameter estimates as accurate as HMC, and is more computationally efficient than HMC.

## 5.2 Poisson Log-Normal Model for Web Traffic Prediction

The co-browsing on one high-traffic site and one client site is commonly related to the click-through of users from the former to the latter. Therefore, the count of co-browsing is a useful indication of the click-through traffic. For any given client website, predicting the high traffic sites that could generate the most traffic is of high commercial interest. Therefore, we consider a Poisson regression model. We choose the co-browsing count of one client website as the outcome  $y_i$  and the log count of the other 95 websites as the predictors  $x_{ij} = \log(x_{ij}^* + 1)$  for  $i = 1, \dots, 59792$  and  $j = 1, \dots, 95$ . A Gaussian random effect is included to account for over-dispersion relative to the Poisson distribution, leading to a Poisson log-normal regression model.

$$\begin{aligned}
 y_i &\sim \text{Poisson}(\exp(x_i\beta + \tau_i)), & \tau_i &\stackrel{iid}{\sim} \text{No}(\tau_0, \nu^2), & i = 1 \dots n \\
 \beta &\sim \text{No}(0, I\sigma_\beta^2), & \tau_0 &\sim \text{No}(0, \sigma_\tau^2) & \nu^2 \sim \pi(\nu^2).
 \end{aligned}$$

We assign a weakly informative prior for  $\beta$  and  $\tau_0$  with  $\sigma_\beta^2 = \sigma_\tau^2 = 100$ . For the over-dispersion parameter  $\nu^2$ , we assign a non-informative uniform prior.



When  $\beta$  and  $\tau$  are sampled separately, the random effects  $\tau = \{\tau_1, \dots, \tau_n\}$  can cause slow mixing. Instead, we sample  $\beta$  and  $\tau$  jointly. Using  $\tilde{X} = [I_n || X]$  as a  $n \times (n + p)$  juxtaposed matrix, and  $\eta_i = x_i\beta + \tau_i$  for the linear predictor, the model can be viewed as a linear predictor with  $n + p$  coefficients, and  $\theta = \{\tau, \beta\}'$  can be sampled jointly in a block. The reason for improved mixing with blocked sampling can be found in Liu (1994a).

We now focus on the mixing behavior of data augmentation. We first review data augmentation for the Poisson log-normal model. Zhou et al. (2012) proposed to treat  $\text{Poisson}(\eta_i)$  as the limit of the negative binomial  $\text{NB}(\lambda, \frac{\eta_i}{\lambda + \eta_i})$  with  $\lambda \rightarrow \infty$ , and used moderate  $\lambda = 1,000$  for approximation. The limit can be simplified as (omitting constant):

$$L(\eta_i; y_i) = \frac{\exp(y_i \eta_i)}{\exp\{\exp(\eta_i)\}} = \lim_{\lambda \rightarrow \infty} \frac{\exp(y_i \eta_i)}{\{1 + \exp(\eta_i)/\lambda\}^\lambda}. \quad (11)$$

With finite  $\lambda$  approximation, the posterior can be sampled via Polya-Gamma augmented Gibbs sampling:

$$\begin{aligned} z_i \mid \eta_i &\sim \text{PG}(\lambda, \eta_i - \log \lambda) \quad i = 1 \dots n \\ \theta \mid z, y &\sim \text{No}\left((\tilde{X}'Z\tilde{X} + \begin{bmatrix} 1/\nu^2 \cdot I_n & 0 \\ 0 & 1/\sigma_\beta^2 \cdot I_p \end{bmatrix})^{-1} \left\{ \tilde{X}'(y - \lambda/2 + Z \log \lambda) + \begin{bmatrix} \tau_0/\nu^2 1_n \\ 0_p \end{bmatrix} \right\}, \right. \\ &\quad \left. (\tilde{X}'Z\tilde{X} + \begin{bmatrix} 1/\nu^2 \cdot I_n & 0 \\ 0 & 1/\sigma_\beta^2 \cdot I_p \end{bmatrix})^{-1} \right), \end{aligned}$$

where  $Z = \text{diag}\{z_1, \dots, z_n\}$ ,  $1_n = \{1, \dots, 1\}'$  and  $0_p = \{0, \dots, 0\}'$ .

However, this approximation-based data augmentation is inherently problematic. For example, setting  $\lambda = 1,000$  leads to large approximation error. As in (11), the approximating denominator has  $(1 + \exp(\eta_i)/\lambda)^\lambda = \exp\{\exp(\eta_i) + \mathcal{O}(\exp(2\eta_i)/\lambda)\}$ ; for moderately large  $\eta_i \approx 10$ ,  $\lambda$  needs to be at least  $10^9$  to make  $\exp(2\eta_i)/\lambda$  close to 0. This large error cannot be corrected with an additional M-H step, since the acceptance rate would be too low. On the other hand, it is not practical to use a large  $\lambda$  in a Gibbs sampler, as it would create extremely large  $z_i$  (associated with small conditional covariance for  $\theta$ ), resulting in slow mixing.

We use CDA to solve this dilemma. We first choose a very large  $\lambda$  ( $10^9$ ) to control the approximation error, then use a small fractional  $r_i$  multiplying to  $\lambda$  for calibration. This leads to a proposal likelihood similar to the logistic CDA:

$$L_{r,b}(x_i \theta; y_i) = \frac{\exp(\eta_i - \log \lambda + b_i)^{y_i}}{\{1 + \exp(\eta_i - \log \lambda + b_i)\}^{r_i \lambda}},$$

with  $r_i \geq (y_i - 1)/\lambda + \epsilon$  for proper likelihood, and proposal update rule:

$$\begin{aligned} z_i &\sim \text{PG}(r_i \lambda, \eta_i - \log \lambda + b_i) \quad i = 1 \dots n \\ \theta^* &\sim \text{No}\left((\tilde{X}'Z\tilde{X} + \begin{bmatrix} 1/\nu^2 \cdot I_n & 0 \\ 0 & 1/\sigma_\beta^2 \cdot I_p \end{bmatrix})^{-1} \left\{ \tilde{X}'(y - r\lambda/2 + Z \log(\lambda - b)) + \begin{bmatrix} \tau_0/\nu^2 1_n \\ 0_p \end{bmatrix} \right\}, \right. \\ &\quad \left. (\tilde{X}'Z\tilde{X} + \begin{bmatrix} 1/\nu^2 \cdot I_n & 0 \\ 0 & 1/\sigma_\beta^2 \cdot I_p \end{bmatrix})^{-1} \right) \end{aligned}$$

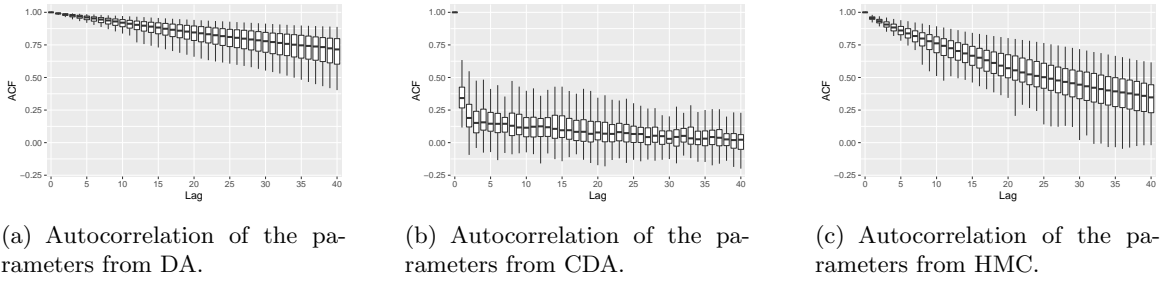
Letting  $\eta_i^* = \tilde{X}\theta^*$ , the proposal is accepted with probability (based on Poisson density and the approximation  $L_{r,b}(x_i\theta; y_i)$ ):

$$1 \wedge \prod_i \frac{\exp\{\exp(\eta_i)\}}{\exp\{\exp(\eta_i^*)\}} \frac{\{1 + \exp(\eta_i^* - \log \lambda + b_i)\}^{r_i \lambda}}{\{1 + \exp(\eta_i - \log \lambda + b_i)\}^{r_i \lambda}}.$$

During the tuning, we set  $r_i = 1/c_0\tau_i \exp(\eta_i) / \left( \frac{\lambda}{2|\eta_i + b_i - \log \lambda|} \tanh \frac{|\eta_i + b_i - \log \lambda|}{2} \right) \vee ((y_i - 1)/\lambda + \epsilon)$  based on the Fisher information. We first found the acceptance rate too low with  $c_0 = 1$ , which indicates an overestimation of the marginal variance; we then reduce  $c_0 = 0.1$  to increase the acceptance rate to a satisfactory 0.6. Conditionally on  $r_i$ , we used  $b_i = \log[\exp\{\exp(\eta_i - \log \lambda - \log r_i)\} - 1] - \eta_i + \log \lambda$ . After  $\theta$  is updated, the other parameters can be sampled via  $\tau_0 \sim \text{No}((n/\nu^2 + 1/\sigma_\tau^2)^{-1} \sum_i \tau_i/\nu^2, (n/\nu^2 + 1/\sigma_\tau^2)^{-1})$  and  $\nu^2 \sim \text{Inverse-Gamma}(n/2 - 1, \sum_i (\tau_i - \tau_0)^2/2)$ .

We ran the basic DA with  $\lambda = 1,000$  approximation, CDA with  $\lambda = 10^9$  and HMC. We ran DA for 200,000 steps, CDA for 2,000 steps and HMC for 20,000 steps so that they have approximately the same effective sample size. For CDA, we used the first 1,000 steps for adapting  $r$  and  $b$ . Figure 6 shows the mixing of DA, CDA and HMC. Even with small  $\lambda = 1,000$  in DA, all of the parameters mix poorly; HMC seemed to be affected by the presence of random effects, and most of parameters remain highly correlated within 40 lags; CDA substantially improves the mixing. Table 2 compares all three algorithms. CDA has the most efficient computing time per effective sample, and is about 30 – 300 times more efficient than the other two algorithms.

Figure 6: CDA significantly improves the mixing of the parameters in the Poisson log-normal.



To evaluate the prediction performance, we use another co-browsing count table for the same high traffic and client sites, collected during a different time period. We use the high traffic co-browsing count  $x_{ij}^{\dagger*}$  and their log transform  $x_{ij}^{\dagger} = \log(x_{ij}^{\dagger*} + 1)$  for the  $j = 1, \dots, 95$  clients to predict the count for the client of interest  $y_i^{\dagger}$ , over the high traffic site  $i = 1, \dots, 59792$ . We carry out prediction using  $\hat{y}_i^{\dagger} = \mathbb{E}_{\beta, \tau | y, x} y_i^{\dagger} = \mathbb{E}_{\beta, \tau | y, x} \exp(x_i^{\dagger} \beta + \tau_i)$  on the client site. The expectation is taken over posterior sample  $\beta, \tau | y, x$  with training set  $\{y, x\}$  discussed above. Cross-validation root-mean-squared error  $(\sum_i (\hat{y}_i^{\dagger} - y_i^{\dagger})^2/n)^{1/2}$  between the prediction and actual count  $y_i^{\dagger}$ 's is computed. Shown in Table 2, slow mixing

in DA and HMC cause poor estimation of the parameters and high prediction error, while CDA has significantly lower error.

	DA	CDA	HMC
$\sum \beta_j / 95$	0.072 (0.071, 0.075)	-0.041 (-0.042, -0.038)	-0.010 (-0.042, -0.037)
$\sum \beta_j^2 / 95$	0.0034 (0.0033, 0.0035)	0.231 (0.219, 0.244)	0.232 (0.216, 0.244)
$\sum \tau_i / n$	-0.405 (-0.642, -0.155)	-1.292 (-2.351, -0.446)	-1.297 (-2.354, -0.451)
$\sum \tau_i^2 / n$	1.126 (0.968, 1.339)	3.608 (0.696, 7.928)	3.589 (0.678, 8.011)
Prediction RMSE	33.21	8.52	13.18
$T_{eff} / T$	0.0037 (0.0011, 0.0096)	0.3348 (0.0279, 0.699)	0.0173 (0.0065, 0.0655)
Avg Computing Time / $T$	1.3 sec	1.3 sec	56 sec
Avg Computing Time / $T_{eff}$	346.4 sec	11.5 sec	3240.6 sec

Table 2: Parameter estimates, prediction error and computing speed of the DA, CDA and HMC in Poisson regression model.

## 6. Discussion

Data augmentation (DA) is a technique routinely used to enable implementation of simple Gibbs samplers, avoiding the need for expensive and complex tuning of Metropolis-Hastings algorithms. Despite the convenience, DA can slow down mixing when the conditional posterior variance given the augmented data is substantially smaller than the marginal variance. When the sample size is massive, this problem arises when the rates of convergence of the augmented and marginal posterior differ, leading to critical mixing problems. There is a very rich literature on strategies for improving mixing rates of Gibbs samplers, with centered or non-centered re-parameterizations (Papaspiliopoulos et al., 2007) and parameter-expansion (Liu and Wu, 1999) leading to some improvements. However, existing approaches have limited ability to solve large sample mixing problems in not addressing the fundamental rate mismatch issue.

To tackle this problem, we propose to calibrate the data augmentation and use a parameter to directly adjust the conditional variance (which is associated with step size). The generated samples are used as a proposal in M-H to obtain the correct posterior. As the original un-calibrated Gibbs sampler is a special case with  $r = 1, b = 0$ , CDA can be viewed as a generalized class of sampling algorithms with data augmentation. CDA adds a little cost due to the likelihood evaluation, which is often negligible as dominated by the random number generation. In this article, we demonstrate that calibration is generally applicable when  $\theta | z$  belongs to the location-scale family. We expect it to be extensible to any conditional distribution with a variance or scale.

As both CDA and HMC involve M-H step, we would like to draw some further comparison between the two. Both methods rely on finding a good proposal by searching a region far from the current state. One key difference lies in the computing efficiency. Although HMC is more generally applicable beyond data augmentation, it is computationally intensive since Hamiltonian dynamics often requires multiple numeric steps. CDA only requires one step of calibrated Gibbs sampling, which is often much more efficient leveraging on existing data augmentation algorithms.

## Appendix A. Appendix

### A.1 Proof of Remark 1

**Proof** Since  $Q_{r,b}(\theta; \theta')$  is the  $\theta$  marginal of a Gibbs transition kernel, and Gibbs is reversible on its margins, we have

$$Q(\theta; \theta')\Pi_{r,b}(\theta) = Q(\theta'; \theta)\Pi_{r,b}(\theta),$$

and so

$$\begin{aligned} \frac{L(\theta'; y)\Pi^0(\theta')Q(\theta; \theta')}{L(\theta; y)\Pi^0(\theta)Q(\theta'; \theta)} &= \frac{L(\theta'; y)\Pi^0(\theta')L_{r,b}(\theta; y)\Pi^0(\theta)}{L(\theta; y)\Pi^0(\theta)L_{r,b}(\theta'; y)\Pi^0(\theta')} \\ &= \frac{L(\theta'; y)L_{r,b}(\theta; y)}{L(\theta; y)L_{r,b}(\theta'; y)}. \end{aligned}$$

■

### A.2 Proof of Remark 2

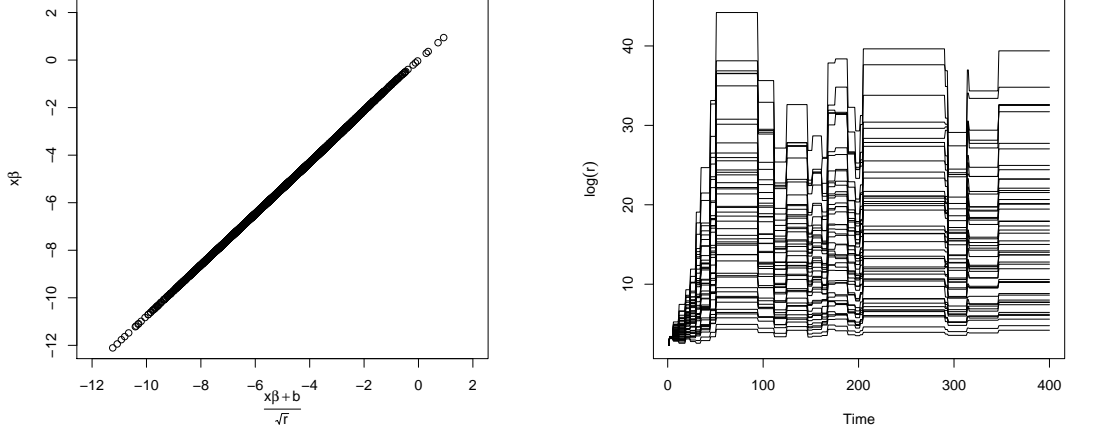
**Proof** For any  $r, b$ , the conditionals  $\Pi_{r,b}(z \mid \theta)$  and  $\Pi_{r,b}(\theta \mid z)$  are well-defined for all  $z \in \mathcal{Z}, \theta \in \Theta$ , and therefore the Gibbs transition kernel  $K_{r,b}((\theta, z); \cdot)$  and corresponding marginal kernels  $Q_{r,b}(\theta; \cdot)$  are well-defined. Moreover, for any  $(z, \theta) \in \mathcal{Z} \times \Theta$ , we have  $\mathbb{P}[(\theta', z') \in A \mid (\theta, z)] > 0$  by assumption. Thus  $K_{r,b}$  is aperiodic and  $\Pi_{r,b}$ -irreducible (see the discussion following Corollary 1 in Roberts and Smith (1994)).

$Q_{r,b}(\theta'; \theta)$  is aperiodic and  $\Pi_{r,b}(\theta)$ -irreducible, since it is the  $\theta$  marginal transition kernel induced by  $K_{r,b}((\theta, z); \cdot)$ . Thus, it is also  $\Pi(\theta)$ -irreducible so long as  $\Pi \gg \Pi_{r,b}$ , where for two measures  $\mu, \nu$ ,  $\mu \gg \nu$  indicates absolute continuity. Since  $\Pi, \Pi_{r,b}$  have densities with respect to Lebesgue measure,  $\Pi_{r,b}$ -irreducibility implies  $\Pi$  irreducibility. Moreover,  $Q(\theta; \theta') > 0$  for all  $\theta \in \Theta$ . Thus, by (Roberts and Smith, 1994, Theorem 3), CDA M-H is  $\Pi$ -irreducible and aperiodic. ■

### A.3 Diagnostics of adaptation

We adapt the tuning parameters  $(r, b)$  by locally solving  $\Delta_{\mathcal{I}-1}(\hat{\theta}_t) = 0$  and optimizing acceptance rate near  $\hat{\theta}_{MAP}$  during adaptation. Updating  $b$  as a function of  $\theta$  yields  $L_{r,b}(\theta; y) = L(\theta; y)$  exactly; after adaptation, for fixed  $(r, b)$ ,  $L_{r,b}(\theta; y)$  is close to  $L(\theta; y)$  for  $\theta$  in the neighborhood around  $\hat{\theta}_{MAP}$ . To show this empirically, consider the probit Bernoulli regression example. As the  $L(\theta; y)$  and  $L_{r,b}(\theta; y)$  are parameterized by  $\Phi(x_i\beta)$  and  $\Phi(\frac{x_i\beta + b_i}{\sqrt{r_i}})$ , Figure 7(a) compares the posterior values of  $x_i\beta$  against  $\frac{x_i\beta + b_i}{\sqrt{r_i}}$ . Clearly, the two are very close with a RMSE of 0.23. Figure 7(b) shows the trace of the adaptation of  $r$  during the initial 400 iterations;  $r$  quickly rise from 1 to the roughly appropriate scale during the initial 50 steps. The values of  $(r, b)$  are fixed afterwards to ensure ergodicity.

Figure 7: Diagnostics plot of the adaptation for probit regression.


 (a) Posterior sample of  $x_i \beta$  and its corresponding transform  $\frac{x_i \beta + b_i}{\sqrt{r_i}}$  in probit CDA.

 (b) Trace of the adaptation of  $r$ , shown on log scale.

#### A.4 Calibrated Polya-Gamma algorithm with sub-sampling

Adapting based on Johndrow et al. (2017), we first randomly sample a subset of indices  $V$  of size  $|V|$ . This algorithm generates proposal from

$$\begin{aligned} V &= V_1 \cup V_0, \quad V_1 = \{i \in \{1, \dots, n\} : y_i = 1\}, \quad V_0 \sim \text{Subset}(|V|, \{i \in \{1, \dots, n\} : y_i = 0\}) \\ z_i &\sim \text{PG}(k_i r_i, |x_i \theta + b_i|) \quad i \in V, \\ \theta^* &\sim \text{No} \left( (X_V' Z_V X_V)^{-1} X_V' (y_V - k_V r_V / 2 - Z_V b_V), (X_V' Z_V X_V)^{-1} \right), \end{aligned}$$

where subscript  $\cdot_V$  indicates the sub-matrix or sub-vector corresponding to the sub-sample;  $k_i = 1$  if  $y_i = 1$ , and  $k_i = \frac{n - |V_1|}{|V_0|}$ . We accept  $\theta^*$  in M-H step using calibrated likelihood

$$L_{r,b}(\theta; y) = \prod_{i \in V_1} \frac{\exp(x_i \theta + b_i)}{\{1 + \exp(x_i \theta + b_i)\}^{r_i}} \left( \prod_{i \in V_0} \frac{1}{\{1 + \exp(x_i \theta + b_i)\}^{r_i}} \right)^{\frac{n - |V_1|}{|V_0|}},$$

with target approximate likelihood  $L_{1,0}(\theta; y)$ . Using Fisher information, the parameters are adapted initially for 200 steps, via  $r_i = \frac{\exp(x_i \theta)}{\{1 + \exp(x_i \theta)\}^2} / \left( \frac{1}{2|x_i \theta + b_i|} \tanh \frac{|x_i \theta + b_i|}{2} \right) \vee ((y_i - 1)/k_i + \epsilon)$  and  $b_i = \log[\{1 + \exp(x_i \theta + b_i)\}^{1/r_i} - 1] - x_i \theta$ .

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