Statistica Sinica Preprint No: SS-2018-0439	
Title	OPTIMAL SUBSAMPLING ALGORITHMS FOR BIG DATA REGRESSIONS
Manuscript ID	SS-2018-0439
URL	http://www.stat.sinica.edu.tw/statistica/
DOI	10.5705/ss.202018.0439
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Notice: Accepted version subject to English editing.	

Statistica Sinica

OPTIMAL SUBSAMPLING ALGORITHMS FOR BIG DATA REGRESSIONS

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Abstract: To fast approximate maximum likelihood estimators with massive data, this paper studies the **o**ptimal **s**ubsampling **m**ethod under the **A**-optimality **c**riterion (OSMAC) for generalized linear models. The consistency and asymptotic normality of the estimator from a general subsampling algorithm are established, and optimal subsampling probabilities under the A- and L-optimality criteria are derived. Furthermore, using Frobenius norm matrix concentration inequalities, finite sample properties of the subsample estimator based on optimal subsampling probabilities are also derived. Since the optimal subsampling probabilities depend on the full data estimate, an adaptive two-step algorithm is developed. Asymptotic normality and optimality of the estimator from this adaptive algorithm are established. The proposed methods are illustrated and evaluated through numerical experiments on simulated and real datasets.

Key words and phrases: generalized linear models; massive data; matrix concen-

tration inequality.

1. Introduction

Nowadays, massive data sets are ubiquitous in many scientific fields and practices such as in astronomy, economics, and industrial problems. Extracting useful information from these large data sets is a core challenge for different communities including computer science, machine learning, and statistics. Over last decades, progresses have been made through various investigations to meet this challenge. However, computational limitations still exist due to the faster growing pace of data volumes. For this, subsampling is a popular technique to extract useful information from massive data. This paper focuses on this technique and will develop optimal subsampling strategies for generalized linear models (GLMs). Typically the maximum likelihood estimators (MLE) are found numerically by using the Newton-Raphson method. However, fitting a GLM on massive data is not an easy task through the iterative Newton-Raphson method, and it requires $O(p^2n)$ time in each iteration of the optimization procedure.

An efficient way to solve this problem is the subsampling method (see Drineas et al., 2006, as an example) as this method essentially downsizes the data volume. Drineas et al. (2011) proposed to make a randomized

Hadamard transform on data and then use uniform subsampling to take random subsamples to approximate ordinary least square estimators in linear regression models. Ma et al. (2015), Ma and Sun (2015) developed an effective subsampling method for linear regression models, which uses normalized statistical leverage scores of the covariate matrix as non-uniform subsampling probabilities. Jia et al. (2014) studied leverage sampling for GLMs based on generalized statistical leverage scores. Wang et al. (2018b) and Yao and Wang (2019) developed an optimal subsampling procedure to minimize the asymptotic mean squared error (MSE) of the resultant subsample-estimator given the full data which is based on A- or L-optimality criterion in the language of optimal design. Wang et al. (2019) proposed a new algorithm called information-based optimal subdata selection method for linear regressions on big data. The basic idea is to select the most informative data points deterministically based on D-optimality without relaying on random subsampling. A divide-and-conquer version of the algorithm was developed in Wang (2019). Recent developments of big data subsampling method can be found in Wang et al. (2016).

Methodological investigations on subsampling methods with statistical guarantees for massive data regression are still limited when models are complex. To the best of our knowledge, most of the existing results con-

cern linear regression models such as in Ma et al. (2015) and Wang et al. (2019). The optimal subsampling method in Wang et al. (2018b) and Yao and Wang (2019) is designed specifically for logistic and multinomial regression models, respectively. However, only linear and logistic regressions are not enough to meet practical needs (Czado and Munk, 2000). For example, we may need Poisson or negative binomial distribution for count data and need Gamma or inverse Gaussian distribution for data with non-negative responses. In addition, the aforementioned investigations did not consider finite sample properties of subsampled estimators. In this paper, we fill these gaps by deriving optimal subsampling probabilities for GLMs, including these with non-canonical link functions which allow for a wide range of statistical models for regression analysis. Furthermore, we will derive finite-sample upper bounds for approximation errors that can be practically used to make the balance between the subsample size and prediction accuracy. Due to the non-natural link, our investigation is substantially distinct from the that in Wang et al. (2018b). For example, the Hessian matrix in the models considered in this paper may be dependent on responses.

The rest of this paper is organized as follows. Section 2 introduces the model setup and derives asymptotic properties for the general subsampling estimator. Section 3 derives optimal subsampling strategies based on A-

and L-optimality criteria for GLMs. Finite-sample error bounds are also derived in this section. Section 4 designs a two-step algorithm to approximate the optimal subsampling procedure and obtains asymptotic properties of the resultant estimator. Section 5 illustrates our methodology through numerical simulations and a real data applications.

2. Preliminaries

2.1 Models and Assumptions

Recall the definition of one parameter exponential family of distributions $f(y|\theta) = h(y)\exp(\theta y - \psi(\theta)), \theta \in \Theta$ as in (5.50) of Efron and Hastie (2016), where θ is called the canonical parameter and Θ is called the natural parameter space. Here $f(\cdot|\theta)$ is a probability density function for the continuous case or a probability mass function for the discrete case; $h(\cdot)$ is a specific function that does not depend on θ; and the parameter space Θ is defined as $\Theta := \{\theta \in \mathbb{R} : \int h(x)\exp(\theta x)\mu(dx) < \infty\}$ with μ being the dominating measure. The exponential family includes most of the commonly used distributions such as normal, gamma, Poisson, and binomial distributions (see Efron and Hastie, 2016; Mccullagh and Nelder, 1989).

A key tactic for a generalized linear regression model is to express θ in form of a linear function of regression coefficients. Let $(\boldsymbol{x}, y)$ be a pair

of random variables where $y \in \mathbb{R}$ and $\boldsymbol{x} \in \mathbb{R}^p$. The generalized linear regression model assumes that the conditional distribution of y_i given $\boldsymbol{x}_i$ is determined by $\theta_i = u(\boldsymbol{\beta}^T \boldsymbol{x}_i)$. Specifically for exponential family, it assumes that the distribution of $y|\boldsymbol{x}$ is

$$f(y|\boldsymbol{\beta}, \boldsymbol{x}) = h(y) \exp(yu(\boldsymbol{\beta}^T \boldsymbol{x}_i) - \psi(u(\boldsymbol{\beta}^T \boldsymbol{x}_i))), \quad \text{with} \quad \boldsymbol{\beta}^T \boldsymbol{x} \in \Theta. \quad (2.1)$$

The problem of interest is to estimate the unknown $\boldsymbol{\beta}$ from observed data. As special case when $u(t) = t$, the corresponding models are the so-called GLMs with canonical link functions. Some typical examples of this type GLMs are logistic regression for binary data and Poisson regression for count data. A commonly used GLM with non-canonical link function is negative binomial regression (NBR), which is often used as an alternative to Poisson regression when data exhibit overdispersion. For this model, $u(t) = t - \log(\nu + e^t)$ and $\psi(u(t)) = \nu \log(\nu + e^t)$ for some size parameter ν.

2.2 General Subsampling Algorithm and its Asymptotic Properties

In this subsection, we study a general subsampling algorithm for GLMs and obtain some asymptotic results.

To facilitate the presentation, denote the full data matrix by $\mathcal{F}_n = (\boldsymbol{X}, \boldsymbol{y})$, where $\boldsymbol{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)^T$ is the covariate matrix and $\boldsymbol{y} = (y_1, \ldots, y_n)^T$

is the response vector. In this paper, we assume that $(\boldsymbol{x}_i, y_i)$'s are independently generated from a GLM. Let S be a set of subsample with r data points, and define the sampling distribution π_i for all data points $i = 1, 2, ...n$ as $\boldsymbol{\pi}$. A general subsampling algorithm follows the steps below.

1. Assign a sampling distribution $\boldsymbol{\pi}$ such that in each draw, the i-th element in the full dataset $\mathcal{F}_n$ has the inclusion probability π_i.

2. Sample with replacement r times to form the subsample set $S := \{(y_i^*, \boldsymbol{x}_i^*, \pi_i^*), i = 1, \ldots, r\}$, where $\boldsymbol{x}_i^*$, y_i^*, and π_i^* stand for covariates, responses, and subsampling probabilities in the subsample, respectively.

3. Based on the subsample set S, calculate the weighted log-likelihood estimator by maximizing the following function

$$L^*(\boldsymbol{\beta}) = \frac{1}{r}\sum_{t=1}^{r}\frac{1}{\pi_i^*}[y_i^* u(\boldsymbol{\beta}^T\boldsymbol{x}_i^*) - \psi(u(\boldsymbol{\beta}^T\boldsymbol{x}_i^*))]. \tag{2.2}$$

An important feature of the above algorithm is that subsample estimator is essentially a weighted MLE and the corresponding weights are inverses of subsampling probabilities. This is analogous to the Hansen-Hurwitz estimator (Hansen and Hurwitz, 1943) in classic sampling techniques. For an overview see Särndal et al. (1992). Although Ma et al. (2015) showed

that the unweighted subsample estimator is asymptotically unbiased for $\boldsymbol{\beta}$ in leveraging sampling, an unweighted subsample estimator is in general biased if the sampling distribution $\boldsymbol{\pi}$ depends on the responses. The inverse-probability weighting scheme is to remove bias, and we restrict our analysis on the weighted estimator here.

Let $\dot{\psi}(t)$ and $\ddot{\psi}(t)$ be the first and the second derivatives of $\psi(t)$, respectively. To characterize asymptotic properties of subsampled estimators, we require some regularity assumptions listed below.

(H.1): Assume that $\boldsymbol{\beta}^T\boldsymbol{x}$ lies in the interior of a compact set $K \in \Theta$ almost surely.

(H.2): The regression coefficient $\boldsymbol{\beta}$ is a inner point of the compact domain $\Lambda_B = \{\boldsymbol{\beta} \in \mathbb{R}^p : \|\boldsymbol{\beta}\| \leq B\}$ for some constant B.

(H.3): Central moments condition: $n^{-1}\sum_{i=1}^{n} |y_i - \dot{\psi}(u(\boldsymbol{\beta}^T\boldsymbol{x}_i))|^4 = O_P(1)$ for all $\boldsymbol{\beta} \in \Lambda_B$.

(H.4): As $n \to \infty$, the observed information matrix

$$\mathcal{J}_X := \tfrac{1}{n}\sum_{i=1}^{n} \{\ddot{u}(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\boldsymbol{x}_i^T[\dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i)) - y_i] + \ddot{\psi}(u(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i))\dot{u}^2(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\boldsymbol{x}_i^T]\}$$

goes to a positive-definite matrix in probability.

(H.5): Require that the full sample covariates have finite 6th-order moments, i.e., $E\|\boldsymbol{x}_1\|^6 \leq \infty$.

(H.6): Assume $n^{-2}\sum_{i=1}^{n}\|\boldsymbol{x}_i\|^k/\pi_i = O_P(1)$ for $k = 2, 4$.

(H.7): For $\gamma = 0$ and some $\gamma > 0$, assume

$$\frac{1}{n^{2+\gamma}}\sum_{i=1}^{n}\frac{|y_i - \dot{\psi}_i(u(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i))|^{2+\gamma}\|\dot{u}(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\|^{2+\gamma}}{\pi_i^{1+\gamma}} = O_P(1).$$

Here, assumptions (H.1) and (H.2) are the set of assumptions used in Clémencon et al. (2014). The set in (H.2) is also called admissible set which premises for consistency estimation for GLMs with full data (see Fahrmeir and Kaufmann, 1985). These two assumptions ensure that $E(y_i|\boldsymbol{x}_i) < \infty$ for all i. Assumption (H.4) imposes a condition on the covariates to make sure that the MLE based on the full dataset is consistent. To obtain the Bahadur representation of the subsampled estimator, (H.3) and (H.5) are needed. Assumptions (H.6) and (H.7) are moment conditions on covariates and sub-sampling probabilities. Assumption (H.7) is required by the Lindeberg-Feller central limit theorem. Specifically for the uniform subsampling with $\pi_i = n^{-1}$ or more generally when $\max_{i=1,\ldots,n}(n\pi_i)^{-1} = O_P(1)$, (H.7) is implied by that $n^{-1}\sum_{i=1}^{n}|y_i - \dot{\psi}_i(u(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i))|^{2+\gamma}\|\dot{u}(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\|^{2+\gamma} = O_P(1)$, which is guaranteed by the conditions that $E|y|^{4+2\gamma} = O(1)$ under (H.1) and (H.5).

The theorem below presents the consistency of the estimator from the subsampling algorithm to the full data MLE.

Theorem 1. *If Assumptions (H.1)–(H.6) hold, then as* $n \to \infty$ *and* $r \to \infty$, $\tilde{\boldsymbol{\beta}}$ *is consistent to* $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ *in conditional probability given* $\mathcal{F}_n$. *Moreover, the rate of convergence is* $r^{-1/2}$. *That is, with probability approaching one, for any* $\epsilon > 0$, *there exist finite* Δ_ϵ *and* r_ϵ *such that*

$$P(\|\tilde{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{\text{MLE}}\| \geq r^{-1/2}\Delta_\epsilon | \mathcal{F}_n) < \epsilon \tag{2.3}$$

for all $r > r_\epsilon$.

Besides consistency, we derive the asymptotic distribution of the approximation error, and prove that the approximation error, $\tilde{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{\text{MLE}}$, is asymptotically normal in conditional distribution.

Theorem 2. *If Assumptions (H.1)–(H.7) hold, then as* $n \to \infty$ *and* $r \to \infty$, *conditional on* $\mathcal{F}_n$ *in probability,*

$$V^{-1/2}(\tilde{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{\text{MLE}}) \longrightarrow N(0, I) \tag{2.4}$$

in distribution, where $V = \mathcal{J}_X^{-1} V_c \mathcal{J}_X^{-1} = O_p(r^{-1})$ *and*

$$V_c = \frac{1}{rn^2} \sum_{i=1}^{n} \frac{\{y_i - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T \boldsymbol{x}_i))\}^2 \dot{u}^2(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T \boldsymbol{x}_i) \boldsymbol{x}_i \boldsymbol{x}_i^T}{\pi_i}. \tag{2.5}$$

3. Optimal Subsampling Strategies

In this section, we will consider how to specify subsampling distribution $\boldsymbol{\pi} = \{\pi_i\}_{i=1}^n$ with theoretical backup.

3.1 Optimal Subsampling Strategies Based on Optimal Design Criteria

Based on A-optimality criterion in the theory of design of experiments (see Pukelsheim, 2006), optimal subsampling is to choose subsampling probabilities such that the asymptotic MSE of $\tilde{\boldsymbol{\beta}}$ is minimized. This idea was proposed in Wang et al. (2018b) and we call the resulting subsampling strategy *mV-optimal*.

Theorem 3. *The subsampling strategy is mV-optimal if the subsampling probability is chosen such that*

$$\pi_i^{\mathrm{mV}} = \frac{|y_i - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i))| \|\mathcal{J}_X^{-1} \dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\|}{\sum_{j=1}^n |y_j - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i))| \|\mathcal{J}_X^{-1} \dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_j)\boldsymbol{x}_j\|}, \ i = 1, 2, ..., n. \tag{3.6}$$

The optimal subsampling probability $\boldsymbol{\pi}^{\mathrm{mV}}$ has a meaningful interpretation from the view-point of optimal design of experiments (Pukelsheim, 2006). Note that under mild condition the "empirical information matrix" $\mathcal{J}_X^e = \frac{1}{n}\sum_{i=1}^n [y_i - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i))]^2 \dot{u}^2(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\boldsymbol{x}_i^T$ and $\mathcal{J}_X$ converge

to the same limit, the Fisher information matrix of model (2.1). This means that $\mathcal{J}_X^e - \mathcal{J}_X = o_P(1)$. Thus, $\mathcal{J}_X$ can be replaced by $\mathcal{J}_X^e$ in $\boldsymbol{\pi}^{\mathrm{mV}}$, because Theorem 2 still holds if $\mathcal{J}_X$ is replaced by $\mathcal{J}_X^e$ in (2.5). Let $\eta_{\boldsymbol{x}_i} = [y_i - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i))]^2 \dot{u}^2(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i \boldsymbol{x}_i^T$, the contribution of the i-th observation to the empirical information matrix, and $\mathcal{J}_{X\boldsymbol{x}_i\alpha}^e = (1-\alpha)\mathcal{J}_X^e + \alpha\eta_{\boldsymbol{x}_i}$, which can be interpreted as a movement of the information matrix in a direction determined by the i-th observation. The directional derivative of $\mathrm{tr}(\mathcal{J}_X^{e\,-1})$ through the direction determined by the ith observation is $F_i = \lim_{\alpha\to 0+} \alpha^{-1}\{\mathrm{tr}(\mathcal{J}_X^{e\,-1}) - \mathrm{tr}(\mathcal{J}_{X\boldsymbol{x}_i\alpha}^{e\,-1})\}$. This directional derivative is used to measure the relative gain in estimation efficiency under the A-optimality by adding the i-th observations into the sample. Thus, the optimal subsampling strategy prefers to select the data points with large values of directional derivatives, i.e., data points that will result in a larger gain under the A-optimality.

The optimal subsampling strategy derived from mV-optimal critria requires the calculation of $\|\mathcal{J}_X^{-1}\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\|$ for $i = 1, 2, ..., n$, which takes $O(np^2)$ time. To reduce the calculating time, Wang et al. (2018b) proposed a modified optimality criterion to minimize $\mathrm{tr}(V_c)$. This criterion essentially is the L-optimality criterion in optimal experimental design (see Pukelsheim, 2006), which is to improve the quality of $\mathcal{J}_X\tilde{\boldsymbol{\beta}}$. It is easy

to see that only $O(np)$ time is needed to calculate the optimal sampling probabilities. We call the resulting subsampling strategy *mVc-optimal*.

Theorem 4. *The subsampling strategy is mVc-optimal if the subsampling probability is chosen such that*

$$\pi_i^{\mathrm{mVc}} = \frac{|y_i - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i))| \|\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\|}{\sum_{j=1}^n |y_j - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_j))| \|\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_j)\boldsymbol{x}_j\|}, \ i = 1, 2, ..., n. \quad (3.7)$$

Note that in order to calculate $\|\mathcal{J}_X^{-1}\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\|$ for $i = 1, 2, ..., n$, we need $O(np^2)$ time while only $O(np)$ time is needed to evaluate $\|\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\|$. Note that $\mathcal{J}_X$ and V_c are nonnegative definite, and $V = \mathcal{J}_X^{-1} V_c \mathcal{J}_X^{-1}$. Simple matrix algebra yields that $\mathrm{tr}(V) = \mathrm{tr}(V_c \mathcal{J}_X^{-2}) \leq \sigma_{\max}(\mathcal{J}_X^{-2})\mathrm{tr}(V_c)$, where $\sigma_{\max}(A)$ denotes the maximum singular value of matrix A. Since $\sigma_{\max}(\mathcal{J}_X^{-2})$ does not depend on $\boldsymbol{\pi}$, minimizing $\mathrm{tr}(V_c)$ minimizes an upper bound of $\mathrm{tr}(V)$. In fact, for two given subsampling strategies $\boldsymbol{\pi}^{(1)}$ and $\boldsymbol{\pi}^{(2)}$, if $V_c(\boldsymbol{\pi}^{(1)}) \leq V_c(\boldsymbol{\pi}^{(2)})$ in the sense of Loewner-ordering, then it follows that $V(\boldsymbol{\pi}^{(1)}) \leq V(\boldsymbol{\pi}^{(2)})$. Thus the alternative optimality criterion greatly reduces the computing time without losing too much estimation accuracy.

Due to the score function for the log-likelihood, it is interesting that π_i^{mVc}'s in Theorem 4 are proportional to $\|\{y_i - \dot{\psi}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\}\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\|$, norms of gradients of the log-likelihood at individual data points evaluated at the full data MLE. This is trying to find the subsample that best approximate the full data score function at the full data MLE.

We now illustrate Theorem 3 and Theorem 4 with some commonly used GLMs. Note that $u(\cdot)$ is the identity function for GLMs with nature link functions such as logistic and Poisson regressions. For logistic regression,

$$\pi_i^{\mathrm{mV}} = \frac{|y_i - p_i| \left\|\mathcal{J}_X^{-1}\boldsymbol{x}_i\right\|}{\sum_{j=1}^n |y_j - p_j| \left\|\mathcal{J}_X^{-1}\boldsymbol{x}_j\right\|}, \qquad \pi_i^{\mathrm{mVc}} = \frac{|y_i - p_i| \left\|\boldsymbol{x}_i\right\|}{\sum_{j=1}^n |y_j - p_j| \left\|\boldsymbol{x}_j\right\|},$$

with $p_i = \exp(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i)/\{1+\exp(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i)\}$ and $\mathcal{J}_X = n^{-1}\sum_{k=1}^n p_k(1-p_k)\boldsymbol{x}_k\boldsymbol{x}_k^T$. These are the same as the results in Wang et al. (2018b). For Poisson regression,

$$\pi_i^{\mathrm{mV}} = \frac{|y_i - \lambda_i| \left\|\mathcal{J}_X^{-1}\boldsymbol{x}_i\right\|}{\sum_{j=1}^n |y_j - \lambda_j| \left\|\mathcal{J}_X^{-1}\boldsymbol{x}_j\right\|}, \qquad \pi_i^{\mathrm{mVc}} = \frac{|y_i - \lambda_i| \left\|\boldsymbol{x}_i\right\|}{\sum_{j=1}^n |y_j - \lambda_j| \left\|\boldsymbol{x}_j\right\|},$$

with $\lambda_i = \exp(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i)$ and $\mathcal{J}_X = n^{-1}\sum_{k=1}^n \exp(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_k)\boldsymbol{x}_k\boldsymbol{x}_k^T$. NBR does not have a canonical link function, and the conditional distribution of the response is modeled by a two-parameter distribution

$$f(y_i|\nu,\mu_i) = \frac{\Gamma(\nu+y_i)}{\Gamma(\nu)y_i!}\left(\frac{\mu_i}{\nu+\mu_i}\right)^{y_i}\left(\frac{\nu}{\nu+\mu_i}\right)^{\nu}, \quad i = 1,2,\ldots,n,$$

where the size parameter ν can be estimated as a nuisance parameter. The optimal subsampling probabilities for NBR with size parameter ν are

$$\pi_i^{\mathrm{mV}} = \frac{|y_i-\mu_i|\left\|\mathcal{J}_X^{-1}\frac{\nu\boldsymbol{x}_i}{\nu+\mu_i}\right\|}{\sum_{j=1}^n |y_j-\mu_j|\left\|\mathcal{J}_X^{-1}\frac{\nu\boldsymbol{x}_j}{\nu+\mu_j}\right\|}, \qquad \pi_i^{\mathrm{mVc}} = \frac{|y_i-\mu_i|\left\|\frac{\nu\boldsymbol{x}_i}{\nu+\mu_i}\right\|}{\sum_{j=1}^n |y_j-\mu_j|\left\|\frac{\nu\boldsymbol{x}_i}{\nu+\mu_j}\right\|},$$

with $\mu_i = \exp(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i)$ and $\mathcal{J}_X = n^{-1}\sum_{k=1}^n\{\nu(\nu+y_i)\mu_i\}/(\nu+\mu_i)^2\boldsymbol{x}_k\boldsymbol{x}_k^T$.

3.2 Non-asymptotic Properties

We derive some finite sample properties of the subsample estimators based on optimal subsampling probabilities $\boldsymbol{\pi}^{\mathrm{mV}}$ and $\boldsymbol{\pi}^{\mathrm{mVc}}$ in this section. Results are presented in forms of excess risks for approximating the mean responses and they hold for fixed r and n without requiring any quantity to go to infinity. These results show factors that affect the approximation accuracy.

Since $\dot{\psi}(u(\boldsymbol{x}_i^T\boldsymbol{\beta}))$ is the conditional expectation of the response y_i given $\boldsymbol{x}_i$, we aim to characterize the quantity of $\tilde{\boldsymbol{\beta}}$ in prediction by examining $\|\dot{\psi}(u(\boldsymbol{X}_d^T\hat{\boldsymbol{\beta}}_{\mathrm{MLE}})) - \dot{\psi}(u(\boldsymbol{X}_d^T\tilde{\boldsymbol{\beta}}))\|$. This quantity is the distance between the estimated conditional mean responses based on the full data and that based on the subsamples. Intuitively, it measures the goodness of fit in using subsample estimator to predict the mean responses. Note that we can always improve the accuracy of the estimator by increasing the subsample size r. Here we want to have a closer look at the effects of different quantities such as covariate matrix and data dimension and the effect of subsample size r on approximation accuracy.

Let $\sigma_{\max}(A)$ and $\sigma_{\min}(A)$ be the maximum and minimum non-zero singular values of matrix A, respectively, $\kappa(A) := \sigma_{\max}(A)/\sigma_{\min}(A)$. Denote $\dot{\psi}(u(\boldsymbol{X}^T\boldsymbol{\beta}))$, the vector whose the i-th element is $\dot{\psi}(u(\boldsymbol{x}_i^T\boldsymbol{\beta}))$ and define $\dot{u}(\boldsymbol{X}^T\boldsymbol{\beta}) := \mathrm{diag}\{\dot{u}(\boldsymbol{x}_1^T\boldsymbol{\beta}), \cdots, \dot{u}(\boldsymbol{x}_n^T\boldsymbol{\beta})\}$. For the estimator $\tilde{\boldsymbol{\beta}}$ obtained from

the algorithm in Section 2 based on the subsampling probabilities, $\boldsymbol{\pi}^{\mathrm{mV}}$ and $\boldsymbol{\pi}^{\mathrm{mVc}}$, the following theorem holds.

Theorem 5. *Let $\tilde{\boldsymbol{X}}$ denotes the design matrix consisting of subsample covariates with each sampled element rescaled by $1/\sqrt{r\pi_i^*}$. Assume that $\sigma^2_{\min}(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\tilde{\boldsymbol{X}}) \geq 0.5\sigma^2_{\min}(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X})$, and both $\sigma_{\max}(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X})/\sqrt{n}$ and $\sigma_{\min}(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X})/\sqrt{n}$ are bounded. For any given $\epsilon \in (0, 1/3)$, with probability at least $1-\epsilon$, we have*

$$\begin{aligned}&\|\dot{\psi}(u(\boldsymbol{X}^T\hat{\boldsymbol{\beta}}_{\mathrm{MLE}})) - \dot{\psi}(u(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}}))\| \\ &\leq 2C_{\dot{u}}[1 + \frac{4\alpha\sqrt{\log(1/\epsilon)}}{\sqrt{r}}]\sqrt{p}\kappa^2(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X})\|[\boldsymbol{y} - \dot{\psi}(u(\boldsymbol{X}^T\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}))]\|. \quad (3.8)\end{aligned}$$

where $\alpha = \kappa(\mathcal{J}_X^{-1})$ for $\boldsymbol{\pi}^{\mathrm{mV}}$ and $\alpha = 1$ for $\boldsymbol{\pi}^{\mathrm{mVc}}$ and $C_{\dot{u}} = \sup_{r\in K\subset\Theta} |\dot{u}(r)|$.

Theorem 5 not only indicates that the accuracy increases with subsample size r, which agrees with the results in Theorem 1, but also enables us to have a closer look at the effects of different quantities such as covariate matrix and data dimension and the effect of subsample size r on approximation accuracy. Heuristically, the condition number of $\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X}$ measures the collinearity of covariates in the full data covariate matrix; p shows the curse of dimensionality; and $\|\boldsymbol{y} - \dot{\psi}(u(\boldsymbol{X}^T\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}))\|$ measures the goodness of fit of the underlying model on the full data.

The result in (3.8) also indicates that we should choose $r \propto p$ to con-

trol the error bound, hence it seems reasonable to choose the subsample size as $r = cp$. This agrees with the recommendation of choosing a sample size as large as 10 times of the number of covariates in Chapman et al. (1994) and Loeppky et al. (2009) for designed experiments. However, for designed experiments, covariate matrices are often orthogonal or close to be orthogonal, so $\kappa(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X})$ is equal or close to 1 in these cases. For the current paper, full data may not be obtained from well designed experiments so $\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X}$ may vary a lot. Thus, $\kappa(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X})$ should also be considered in determining required subsample size for a given level of prediction accuracy.

The particular constant 0.5 in Theorem 5's condition $\sigma^2_{\min}(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\tilde{\boldsymbol{X}}) \geq 0.5\sigma^2_{\min}(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X})$ can be replaced by any constant between 0 and 1. Here we follow the setting of Drineas et al. (2011) and choose 0.5 for convenience. This condition indicates that the rank of $\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\tilde{\boldsymbol{X}}$ is the same as that of $\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X}$. More details and interpretations about this condition can be found in Mahoney (2012).

Using similar argument as in the proof of Theorem 5, it is proved that this condition holds with high probability.

Theorem 6. *Let $\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\tilde{\boldsymbol{X}}$ denote the design matrix consisting of subsamples with each sampled element rescaled by $1/\sqrt{r\pi_i^*}$. Assume that $|y_i -$*

$\dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i))|\|\dot{u}(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\| \geq \gamma\|\boldsymbol{x}_i\|$ for all i and $\sigma_{\max}(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X})/\sqrt{n}$, $\sigma_{\min}(\dot{u}(\boldsymbol{X}^T\boldsymbol{\beta})\boldsymbol{X})/\sqrt{n}$ are bounded. For any given $\epsilon \in (0, 1/3)$, let $c_d \leq 1$ be a constant depending on $\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X}$, $C_{\dot{u}} = \sup_{r\in K\subset\Theta} |\dot{u}(r)|$ and $r > 64c_d^2C_{\dot{u}}^2\log(1/\epsilon)\sigma_{\max}^4(\boldsymbol{X})p^2/(\alpha^2\delta^2\sigma_{\min}^4(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X}))$ where δ is some constant depending on γ and $\|[\boldsymbol{y} - \dot{\psi}(u(\boldsymbol{X}^T\hat{\boldsymbol{\beta}}_{\text{MLE}}))]\|$. Then with probability at least $1-\epsilon$:

$$\sigma_{\min}^2(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\tilde{\boldsymbol{X}}) \geq 0.5\sigma_{\min}^2(\dot{u}(\boldsymbol{X}^T\tilde{\boldsymbol{\beta}})\boldsymbol{X}),$$

where $\alpha = \kappa(\mathcal{J}_X^{-1})$ for $\boldsymbol{\pi}^{\text{mV}}$ and $\alpha = 1$ for $\boldsymbol{\pi}^{\text{mVc}}$.

4. Practical Consideration and Implementation

For practical implementation, the optimal subsampling probabilities π_i^{mV}'s and π_i^{mVc}'s cannot be used directly because they depend on the unknown full data MLE, $\hat{\boldsymbol{\beta}}_{\text{MLE}}$. As suggested in Wang et al. (2018b), in order to calculate $\boldsymbol{\pi}^{\text{mV}}$ or $\boldsymbol{\pi}^{\text{mVc}}$, a pilot estimator of $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ has to be used. Let $\tilde{\boldsymbol{\beta}}_0$ be a pilot estimator based on a subsample of size r_0. It can be used to replace $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ in $\boldsymbol{\pi}^{\text{mV}}$ or $\boldsymbol{\pi}^{\text{mVc}}$, which then can be used to sample more informative subsamples.

From the expression of $\boldsymbol{\pi}^{\text{mV}}$ or $\boldsymbol{\pi}^{\text{mVc}}$, the approximated optimal subsampling probabilities are both proportional to $|y_i - \dot{\psi}(u(\tilde{\boldsymbol{\beta}}_0^T\boldsymbol{x}_i))|$, so data points with $y_i \approx \dot{\psi}(u(\tilde{\boldsymbol{\beta}}_0^T\boldsymbol{x}_i))$ have very small probabilities to be selected and

data points with $y_i = \dot{\psi}(u(\tilde{\boldsymbol{\beta}}_0^T \boldsymbol{x}_i))$ will never be included in a subsample. On the other hand, if these data points are included in the subsample, the weighted log-likelihood function in (2.2) may be dominated by them. As a result, the subsample estimator may be sensitive to these data points. Ma et al. (2015) also noticed the problem that some extremely small subsampling probabilities may inflate the variance of the subsampling estimator in the context of leveraging sampling.

To protect the weighted log-likelihood function from being inflated by these data points in practical implementation, we propose to set a threshold, say δ, for $|y_i - \dot{\psi}(u(\tilde{\boldsymbol{\beta}}_0^T \boldsymbol{x}_i))|$, i.e., use $\max\{|y_i - \dot{\psi}(u(\tilde{\boldsymbol{\beta}}_0^T \boldsymbol{x}_i))|, \delta\}$ to replace $|y_i - \dot{\psi}(u(\tilde{\boldsymbol{\beta}}_0^T \boldsymbol{x}_i))|$. Here, δ is a small positive number, say 10^{-6} as an example. Setting a threshold δ in subsampling probabilities results in a truncation in the weights for the subsample weighted log-likelihood. Truncating the weight function is a commonly used technique in practice for robust estimation. Note that in practical application, an intercept should always be included in a model, so it is typical that $\|\dot{u}(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\|$ and $\|\mathcal{J}_X^{-1}\dot{u}(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T \boldsymbol{x}_i)\boldsymbol{x}_i\|$ are bounded away from 0 and we do not need to set a threshold for them. Let $\tilde{V}$ be the version of V with $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ substituted by

$\tilde{\boldsymbol{\beta}}_0$. It can be shown that

$$\mathrm{tr}(\tilde{V}) \leq \mathrm{tr}(\tilde{V}^{\delta}) \leq \mathrm{tr}(\tilde{V}) + \frac{\delta^2}{n^2 r} \sum_{i=1}^{n} \frac{1}{\pi_i} \|\tilde{\mathcal{J}}_X^{-1} \dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T \boldsymbol{x}_i) \boldsymbol{x}_i\|^2.$$

Thus, minimizing $\mathrm{tr}(\tilde{V}^{\delta})$ is close to minimizing $\mathrm{tr}(\tilde{V})$ if δ is sufficiently small. The threshold δ is to make our subsampling estimator more robust without scarifying the estimation efficiency too much. Here, we can also approximate $\mathcal{J}_X$ by using the pilot sample. To be specific, the $\mathcal{J}_X$ in mV is approximated by $\tilde{\mathcal{J}}_X = (r_0)^{-1} \sum_{i=1}^{r_0} \{\ddot{u}(\tilde{\boldsymbol{\beta}}^T \boldsymbol{x}_i^*) \boldsymbol{x}_i^* \boldsymbol{x}_i^{*T} [\dot{\psi}(u(\tilde{\boldsymbol{\beta}}^T \boldsymbol{x}_i{}^*)) - y_i{}^*] + \ddot{\psi}(u(\tilde{\boldsymbol{\beta}}^T \boldsymbol{x}_i{}^*)) \dot{u}^2(\tilde{\boldsymbol{\beta}}^T \boldsymbol{x}_i{}^*) \boldsymbol{x}_i{}^* \boldsymbol{x}_i^{*T}]\}$ based on the first stage subsamples $\{(\boldsymbol{x}_i^*, y_i^*) : i = 1, \ldots, r_0\}$.

For transparent presentation, we combine all the aforementioned practical considerations in this section and present a two-step algorithm as below.

1. Run the general subsampling algorithm with $\boldsymbol{\pi} = \boldsymbol{\pi}^{\mathrm{UNIF}}$ and $r = r_0$ to get the pilot subsample set $\tilde{S}_{r_0}$ and a pilot estimator $\tilde{\boldsymbol{\beta}}_0$.

2. Using $\tilde{\boldsymbol{\beta}}_0$ to calculate approximated subsampling probabilities $\tilde{\boldsymbol{\pi}}^{\mathrm{opt}} = \{\tilde{\pi}_i^{\mathrm{mV}}\}_{i=1}^n$ or $\tilde{\boldsymbol{\pi}}^{\mathrm{opt}} = \{\tilde{\pi}_i^{\mathrm{mVc}}\}_{i=1}^n$, where $\tilde{\pi}_i^{\mathrm{mV}}$s are proportional to $\max(|y_i - \dot{\psi}(u(\tilde{\boldsymbol{\beta}}_0^T \boldsymbol{x}_i))|, \delta) \|\tilde{\mathcal{J}}_X^{-1} \dot{u}(\tilde{\boldsymbol{\beta}}_0^T \boldsymbol{x}_i) \boldsymbol{x}_i\|$s and $\tilde{\pi}_i^{\mathrm{mVc}}$s are proportional to $\max(|y_i - \dot{\psi}(u(\tilde{\boldsymbol{\beta}}_0^T \boldsymbol{x}_i))|, \delta) \|\dot{u}(\tilde{\boldsymbol{\beta}}_0^T \boldsymbol{x}_i) \boldsymbol{x}_i\|$.

3. Sample with replacement for r times based on $\tilde{\boldsymbol{\pi}}^{\mathrm{opt}}$ to form the subsample set $S_{r^*} := \tilde{S}_{r_0} \cup \{(y_i^*, \boldsymbol{x}_i^*, \tilde{\pi}_i^*), i = 1, \ldots, r\}$.

4. Maximize the following weighted log-likelihood function to obtain the estimator $\breve{\boldsymbol{\beta}}$

$$L^*(\boldsymbol{\beta}) = \frac{1}{r + r_0} \sum_{i \in S_{r^*}} \frac{1}{\tilde{\pi}_i^*} [y_i^* u(\boldsymbol{\beta}^T \boldsymbol{x}_i^*) - \psi(u\boldsymbol{\beta}^T \boldsymbol{x}_i^*))]. \tag{4.9}$$

We have the following theorems describing asymptotic properties of $\breve{\boldsymbol{\beta}}$.

Theorem 7. *Under Assumptions (H.1)–(H.5), if* $r_0 r^{-1} \to 0$ *as* $r_0 \to \infty, r \to \infty$ *and* $n \to \infty$*, then for the estimator* $\breve{\boldsymbol{\beta}}$ *obtained from the two-step algorithm, with probability approaching one, for any* $\epsilon > 0$*, there exist finite* Δ_ϵ *and* r_ϵ *such that*

$$P(\|\breve{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{\text{MLE}}\| \geq r^{-1/2} \Delta_\epsilon | \mathcal{F}_n) < \epsilon$$

for all $r > r_\epsilon$.

The result of asymptotic normality is presented in the following theorem.

Theorem 8. *Under assumptions (H.1)–(H.5), if* $r_0 r^{-1} \to 0$*, then for the estimator obtained from the two-step algorithm, as* $r_0 \to \infty$*,* $r \to \infty$ *and* $n \to \infty$*, conditional on* $\mathcal{F}_n$*,*

$$V_{opt}^{-1/2} (\breve{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{\text{MLE}}) \to N(0, I), \tag{4.10}$$

where $V_{opt} = \mathcal{J}_X^{-1} V_{c,opt} \mathcal{J}_X^{-1}$*; and*

$$V_{c,opt} = \frac{1}{r} \frac{1}{n} \sum_{i=1}^{n} \frac{\{y_i - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T \boldsymbol{x}_i))\}^2 \dot{u}^2(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T \boldsymbol{x}_i) \boldsymbol{x}_i \boldsymbol{x}_i^T}{\max(|y_i - \dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T \boldsymbol{x}_i))|, \delta) \|\dot{u}(\hat{\boldsymbol{\beta}}_{\text{MLE}}^T \boldsymbol{x}_i) \boldsymbol{x}_i\|} \tag{4.11}$$

$$\times \frac{1}{n}\sum_{i=1}^{n}\max(|y_i-\dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i))|,\delta)\|\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\|,$$

for subsampling probabilities based on $\tilde{\pi}_i^{\mathrm{mVc}}$*, and*

$$V_{c,opt}=\frac{1}{r}\frac{1}{n}\sum_{i=1}^{n}\frac{\{y_i-\dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i))\}^2\dot{u}^2(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\boldsymbol{x}_i^T}{\max(|y_i-\dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i))|,\delta)\|\mathcal{J}_X^{-1}\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\|}$$
$$\times \frac{1}{n}\sum_{i=1}^{n}\max(|y_i-\dot{\psi}(u(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i))|,\delta)\|\mathcal{J}_X^{-1}\dot{u}(\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}^T\boldsymbol{x}_i)\boldsymbol{x}_i\|.$$

for subsampling probabilities based on $\tilde{\pi}_i^{\mathrm{mV}}$*.*

In order to get standard error of the corresponding estimator, we estimate the variance-covariance matrix of $\breve{\boldsymbol{\beta}}$ by $\breve{V}=\breve{\mathcal{J}}_X^{-1}\breve{V}_c\breve{\mathcal{J}}_X^{-1}$, where

$$\breve{\mathcal{J}}_X=\frac{1}{n(r_0+r)}\times$$
$$\Bigg\{\sum_{i=1}^{r_0}\frac{\ddot{u}(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_i^*)\boldsymbol{x}_i^*\boldsymbol{x}_i^T[\dot{\psi}(u(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_i^*))-y_i^*]+\ddot{\psi}(u(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_i^*))\dot{u}^2(\tilde{\boldsymbol{\beta}}_0^T\boldsymbol{x}_i^*)\boldsymbol{x}_i^*\boldsymbol{x}_i^T}{\pi_{i0}^*}$$
$$+\sum_{s=1}^{r}\frac{\ddot{u}(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_s^*)\boldsymbol{x}_s^*\boldsymbol{x}_s^T[\dot{\psi}(u(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_s^*))-y_s^*]+\ddot{\psi}(u(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_s^*))\dot{u}^2(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_s^*)\boldsymbol{x}_s\boldsymbol{x}_s^T}{\tilde{\pi}_s^*}\Bigg\},$$
$$\breve{V}_c=\frac{1}{n^2(r_0+r)^2}\Bigg\{\sum_{i=1}^{r_0}\frac{\{y_i-\dot{\psi}(u(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_i^*))\}^2\dot{u}^2(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_i^*)\boldsymbol{x}_i^*(\boldsymbol{x}_i^*)^T}{(\tilde{\pi}_{i0}^*)^2}$$
$$+\sum_{i=1}^{r}\frac{\{y_i^*-\dot{\psi}(u(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_i^*))\}^2\dot{u}^2(\breve{\boldsymbol{\beta}}^T\boldsymbol{x}_i^*)\boldsymbol{x}_i^*(\boldsymbol{x}_i^*)^T}{(\tilde{\pi}_i^*)^2}\Bigg\},$$

π_{i0}^*'s are the subsampling probabilities used in the first stage, and $\tilde{\pi}_i^*=\tilde{\pi}_i^{\mathrm{mV}*}$ or $\tilde{\pi}_i^{\mathrm{mVc}*}$ for $i=1,\ldots,r$.

5. Numerical Studies

5.1 Simulation Studies

In this section, we use simulation to evaluate the finite sample performance of the proposed method in Poisson regression and NBR. Computations are performed in `R` (R Core Team, 2018). The performance of a sampling strategy $\boldsymbol{\pi}$ is evaluated by the empirical mean squared error (eMSE) of the resultant estimator: $\text{eMSE} = K^{-1}\sum_{k=1}^{K}\|\boldsymbol{\beta}_{\boldsymbol{\pi}}^{(k)} - \hat{\boldsymbol{\beta}}_{\text{MLE}}\|$, where $\boldsymbol{\beta}_{\boldsymbol{\pi}}^{(k)}$ is the estimator from the k-th subsample with subsampling probability $\boldsymbol{\pi}$ and $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ is the MLE calculated from the whole dataset.We set $K = 1000$ throughout this section.

Poisson regression. Full data of size $n = 10,000$ are generated from model $y|\boldsymbol{x} \sim \mathcal{P}(\exp(\boldsymbol{\beta}^T\boldsymbol{x}))$ with the true value of $\boldsymbol{\beta}$ being a 7×1 vector of 0.5. We consider the following four cases to generate the covariates $\boldsymbol{x}_i = (x_{i1}, ..., x_{i7})^T$.

Case 1: The seven covariates are independent and identically distributed (i.i.d) from the standard uniform distribution, namely, $x_{ij} \overset{\text{i.i.d}}{\sim} U([0,1])$ for $j = 1, ..., 7$.

Case 2: The first two covariates are highly correlated. Specifically, $x_{ij} \overset{\text{i.i.d}}{\sim} U([0,1])$ for all j except for $x_{i2} = x_{i1} + \varepsilon_i$ with $\varepsilon_i \overset{\text{i.i.d}}{\sim} U([0, 0.1])$.

For this setup, the correlation coefficient between the first two covariates are about 0.8.

Case 3: This case is the same as the second one except that $\varepsilon_i \overset{\text{i.i.d}}{\sim} U([0,1])$. For this case, the correlation between the first two covariates is close to 0.5.

Case 4: This case is the same as the third one except that $x_{ij} \overset{\text{i.i.d}}{\sim} U([-1,1])$ for $j = 6, 7$. For this case, the bounds for each covariates are not all the same.

We consider both $\tilde{\pi}_i^{\text{mV}}$ and $\tilde{\pi}_i^{\text{mVc}}$, and choose the value of δ to be $\delta = 10^{-6}$. For comparison, we also consider uniform subsampling, i.e., $\pi_i = 1/n$ for all i and the leverage subsampling strategy in Ma et al. (2015)in which $\pi_i = h_i / \sum_{j=1}^{n} h_i = h_i/p$ with $h_i = \boldsymbol{x}_i(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{x}_i$. Here h_i's are the leverage scores for linear regression. For GLMs, leverage scores are defined by using the adjusted covariate matrix, namely, $\tilde{h}_i = \tilde{\boldsymbol{x}}_i(\tilde{\boldsymbol{X}}^T\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{x}}_i$, where $\tilde{\boldsymbol{X}} = (\tilde{\boldsymbol{x}}_1, ..., \tilde{\boldsymbol{x}}_n)^T$, $\tilde{\boldsymbol{x}}_i = \sqrt{-E\{\partial^2 \log f(y_i|\tilde{\theta}_i)/\partial\theta^2\}}\boldsymbol{x}_i$, and $\tilde{\theta}_i = \tilde{\boldsymbol{\beta}}^T\boldsymbol{x}_i$ with an initial estimate $\tilde{\boldsymbol{\beta}}_0$ (see Lee, 1987). In this example, simple algebra yields $\tilde{\boldsymbol{x}}_i = \sqrt{\exp(\tilde{\boldsymbol{\beta}}_0^T\boldsymbol{x}_i)}\boldsymbol{x}_i$. For the leverage score subsampling, we considered both h_i and $\tilde{h}_i$. Here is a summary for the methods to be compared: UNIF, uniform subsample; mV, $\pi_i = \tilde{\pi}_i^{\text{mV}}$; mVc, $\pi_i = \tilde{\pi}_i^{\text{mVc}}$; Lev, leverage sampling

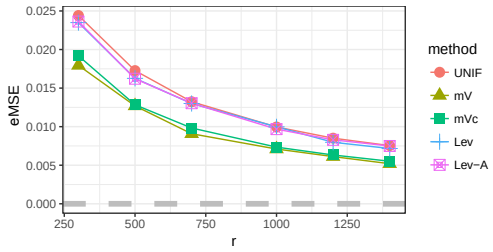
based on h_i; Lev-A, adjust leverage sampling based on $\tilde{h}_i$.

We first consider the case with the first step sample size fixed. We let $r_0 = 200$, and second step sample size r be 300, 500, 700, 1000, 1200 and 1400, respectively. For subsampling probabilities that do not depend on unknown parameters, they are implemented with subsample size $r + r_0$ for fair comparisons.

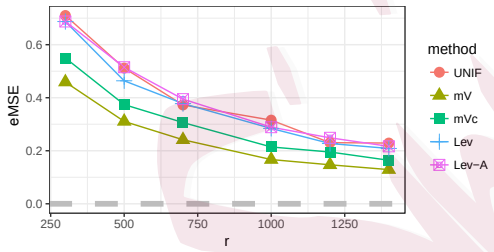
Figure 1 gives eMSEs. It is seen that for all the four data sets, subsampling methods based on $\tilde{\boldsymbol{\pi}}^{\mathrm{mV}}$ and $\tilde{\boldsymbol{\pi}}^{\mathrm{mVc}}$ always result in smaller eMSE than the uniform subsampling, which agrees with the theoretical result that they aim to minimize the asymptotic eMSEs of the resultant estimator. If the components of $\boldsymbol{x}$ are independent, $\tilde{\boldsymbol{\pi}}^{\mathrm{mV}}$ and $\tilde{\boldsymbol{\pi}}^{\mathrm{mVc}}$ have similar performances, while they may perform differently if some covariates are highly correlated. The reason is that $\tilde{\boldsymbol{\pi}}^{\mathrm{mVc}}$ reduces the impact of the data correlation structure since $\|\tilde{\mathcal{J}}_X^{-1}\boldsymbol{x}_i\|^2$ in $\tilde{\boldsymbol{\pi}}^{\mathrm{mV}}$ are replaced by $\|\boldsymbol{x}_i\|^2$ in $\tilde{\boldsymbol{\pi}}^{\mathrm{mVc}}$.

For Cases 1, 3 and 4, eMSEs are small. This is because the condition number of $\boldsymbol{X}_d$ is quite small (≈ 5) and a small subsample size $r = 100$ produces satisfactory results. However, for Case 2, the condition number is large (≈ 40), so a larger subsample size is needed to approximate $\hat{\boldsymbol{\beta}}_{\mathrm{MLE}}$ accurately. This agrees with the conclusion in Theorem 5.

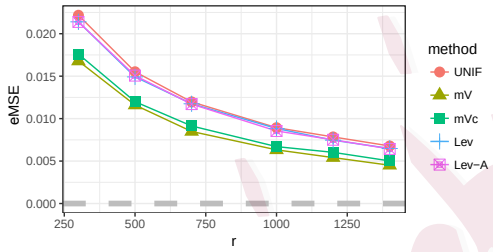
Another contribution of Theorem 8 is to enable us to do inference on



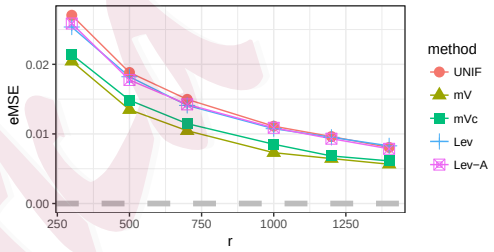
(a) Case 1 (independent covariates)



(b) Case 2 (highly correlated covariates)



(c) Case 3 (weakly correlated covariates)



(d) Case 4 (unequal bounds of covariates)

Figure 1: The eMSEs for Poisson regression with different second step subsample size r and a fixed first step subsample size $r_0 = 200$. The different distributions of covariates are listed in the beginning of Section 5.

$\boldsymbol{\beta}$. Note that in subsampling setting, r is much smaller than the full data size n. If $r = o(n)$, then $\hat{\boldsymbol{\beta}}_{\text{MLE}}$ in Theorem 8 can be replaced by the true parameter. As an example, we take β_2 as a parameter of interest and construct 95% confidence intervals for it. For this, the estimator given by $\breve{V} = \breve{\mathcal{J}}_X^{-1}\breve{V}_c\breve{\mathcal{J}}_X^{-1}$, is used to estimate variance-covariance matrices based on selected subsamples. For comparison, uniform subsampling method is also implemented.

Table 1 reports empirical coverage probabilities and average lengths in Poisson regression model over the four synthetic data sets with the first step subsample size being fixed at $r_0 = 200$. It is clear that $\tilde{\boldsymbol{\pi}}^{\text{mV}}$ and $\tilde{\boldsymbol{\pi}}^{\text{mVc}}$ have similar performances and are uniformly better than the uniform subsampling method. As r increases, the lengths of confidence intervals decrease uniformly which echos the results of Theorem 8. Confidence intervals in Case 2 are longer than those in other cases with the same subsample sizes. This is due to the fact that the condition number of $\boldsymbol{X}_d$ in Case 2 is bigger than that of $\boldsymbol{X}_d$ in other cases. This indicates that we should select a larger subsample when the condition number of the full dataset is bigger, which echoes the results discussed in Section 3.2.

Negative Binomial Regression. We also perform simulation for the negative binomial regression with $n = 100,000$ and summarize the results in

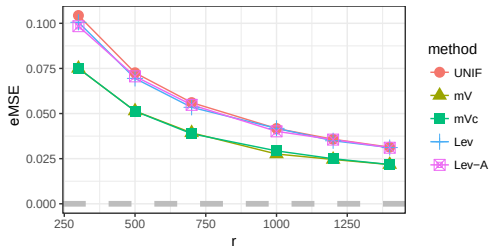
Table 1: Empirical coverage probabilities and average lengths of confidence intervals for β_2. The first step subsample size is fixed at $r_0 = 200$.

	method	mV		mVc		UNIF	
	r	Coverage	Length	Coverage	Length	Coverage	Length
case 1	300	0.954	0.2037	0.955	0.2066	0.952	0.2275
	500	0.954	0.1684	0.945	0.1713	0.942	0.1924
	1000	0.946	0.1254	0.938	0.1281	0.953	0.1471
case 2	300	0.961	1.9067	0.946	2.0776	0.950	2.2549
	500	0.958	1.5470	0.948	1.7263	0.947	1.9082
	1000	0.954	1.1379	0.948	1.2919	0.945	1.4559
case 3	300	0.959	0.1770	0.953	0.1816	0.939	0.2000
	500	0.942	0.1451	0.949	0.1507	0.942	0.1693
	1000	0.954	0.1082	0.954	0.1132	0.939	0.1291
case 4	300	0.955	0.2097	0.951	0.2179	0.953	0.2402
	500	0.951	0.1721	0.956	0.1803	0.942	0.2033
	1000	0.957	0.1276	0.960	0.1347	0.943	0.1552

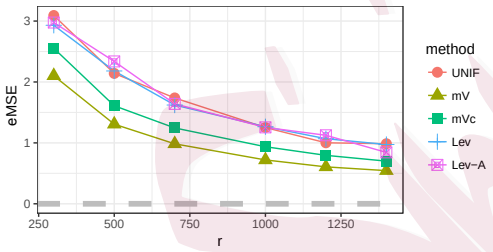
Figure 2. Here we assume $y_i|\boldsymbol{x}_i \sim \mathrm{NB}(\mu_\mathrm{i}, \nu), \quad \mu_\mathrm{i} = \exp(\boldsymbol{\beta}^\mathrm{T}\mathrm{x_i})$ with the size parameter $\nu = 2$. Other simulation settings are the same as the Poisson regression example. It is worthy to mention that compared with Poison regression the eMSE's are lager for NBR when r is the same. This also coincides with Theorem 5 since $C_{\dot{u}} > 1$ for NBR. Result for 95% confidence intervals of β_2 are also reported in Table 2.

Now we investigate the effect of different sample size allocations between the two steps. Since the results for Poisson and NBR have similar performances, we only report the results for Poisson regression to save space. Here, we calculate eMSEs for various proportions of first step subsamples with fixed total subsample sizes. The results are given in Figure 3 with total subsample size $r_0 + r = 800$ and 1200, respectively. Since results are similar for all the cases, we only present results for Case 4 here. It is worthy noting that the two-step method outperforms the uniform subsampling method for all the four cases for both Poisson and NBR, when $r_0/r \in [0.1, 0.9]$. This indicates that the two-step approach is more efficient than the uniform subsampling. The two-step approach works the best when r_0/r is around 0.2.

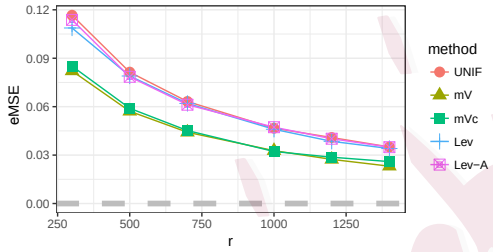
To explore the influence of δ in $\tilde{\pi}_i^{\mathrm{mV}}$ and $\tilde{\pi}_i^{\mathrm{mVc}}$, we calculate eMSEs for various δ ranging from 10^{-6} to 1 with fixed total subsample sizes. Since



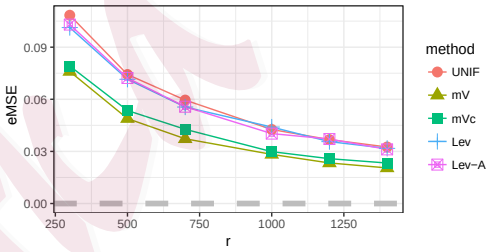
(a) Case 1 (independent covariates)



(b) Case 2 (highly correlated covariates)



(c) Case 3 (weakly correlated covariates)

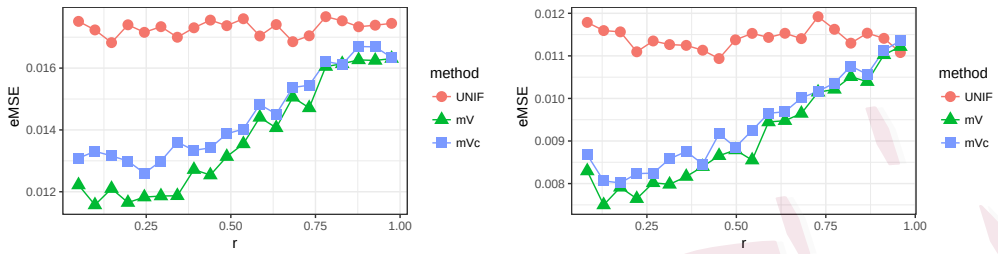


(d) Case 4 (unequal bounds of covariates)

Figure 2: The eMSEs for NBR with different second step subsample size r and a fixed first step subsample size $r_0 = 200$. The different distributions of covariates are listed in the beginning of Section 5.

Table 2: Empirical coverage probabilities and average lengths of confidence intervals for β_2 in NBR with $\nu = 2$. The first step subsample size is fixed at $r_0 = 200$.

	method	mV		mVc		UNIF	
	r	Coverage	Length	Coverage	Length	Coverage	Length
	300	0.952	0.2122	0.955	0.2147	0.947	0.2354
case1	500	0.952	0.1758	0.954	0.1776	0.946	0.1991
	1000	0.951	0.1305	0.933	0.1331	0.940	0.1520
	300	0.947	2.0228	0.963	2.2160	0.943	2.3913
case2	500	0.953	1.6468	0.952	1.8423	0.946	2.0225
	1000	0.957	1.2065	0.947	1.3849	0.942	1.5439
	300	0.950	0.1878	0.950	0.1925	0.942	0.2110
case3	500	0.949	0.1546	0.954	0.1595	0.944	0.1786
	1000	0.953	0.1150	0.957	0.1197	0.943	0.1361
	300	0.956	0.2288	0.953	0.2366	0.953	0.2573
case4	500	0.968	0.1876	0.963	0.1956	0.936	0.2176
	1000	0.950	0.1396	0.952	0.1469	0.940	0.1662

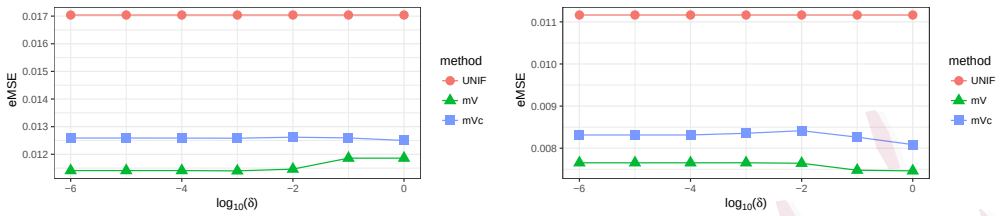


(a) Case 4 ($r_0 + r = 800$) (b) Case 4 ($r_0 + r = 1200$)

Figure 3: The eMSEs vs proportions of the first step subsample with fixed total subsample sizes $r + r_0$ in Poisson regression.

the results for Poisson and NBR are similar, we only report the results for Poisson regression here. Figure 4 presents the results for Case 4 with total subsample size $r_0 + r = 800$ and 1200, respectively. Judging from Figure 4, we see that the eMSE is not sensitive to the choice of δ when δ is not big, say $\delta = 1$ for instance.

To evaluate the computational efficiency of the subsampling strategies, we record the computing times of the five subsampling strategies (uniform, π^{mV}, π^{mVc}, leverage score and adjust leverage score) by using `Sys.time()` function in R to record start and end times of the corresponding code. Each subsampling strategy has been evaluated 50 times. All methods are implemented with the R programming language. Computations were car-



(a) Case 4 ($r_0 + r = 800$) (b) Case 4 ($r_0 + r = 1200$)

Figure 4: The eMSEs vs δ ranging from 10^{-6} to 1 with fixed total subsample sizes $r + r_0$ in Poisson regression. Logarithm is taken on δ for better presentation.

ried out on a desktop running Window 10 with an Intel I7 processor and 32GB memory. Table 3 shows the results for Case 4 with different r and a fixed $r_0 = 400$. The computing time for using the full data is also given for comparisons.

It is not surprising to observe that the uniform subsampling algorithm requires the least computing time because it does not require an additional step to calculate the subsampling probability. The algorithm based on $\boldsymbol{\pi}^{\mathrm{mV}}$ requires longer computing time than the algorithm based on $\boldsymbol{\pi}^{\mathrm{mVc}}$, which agrees with the theoretical analysis in Section 4. The leverage score sampling takes nearly the same time as the mV method since leverage scores are computed directly by the definition. Note that $p = 7$ is not

big enough to use the fast computing method mentioned in Drineas et al. (2011). For fairness, we also consider the case with $p = 80, n = 100,000$, which is suitable to use the fast computing method for the Lev and Lev-A methods. The first seven variables are generated as Case 4 and the rest are generated independently from $U([0,1])$. Here r_0 is also selected as 400 and the corresponding results are reported in Table 5. In order to see the estimation effects we also present eMSEs in Tables 4 and 6, respectively.

From Table 5 it is clear that all the subsampling algorithms take significantly less computing time compared to the full data approach. The Lev and Lev-A are faster than the mV method since the fast algorithm runs in $O(pn \log n)$ time to get the subsampling probabilities, as opposed to the $O(p^2 n)$ time required by the mV method. However, the mVc method is still faster than Lev and Lev-A since the time complexity is just $O(pn)$ in computing the subsampling probabilities. As the dimension increases, the computational advantage of $\boldsymbol{\pi}^{\mathrm{mVc}}$ is even more significant.

5.2 Real Data Studies

In the following, we illustrate our methods described in Section 4 by applying them to a data set from musicology. This data set contains 1,019,318 unique users' music play counts in the Echo Nest which is available at

Table 3: Computing time (in second) for Poisson regression in Case 4 with different r and a fixed $r_0 = 400$.

r	FULL	UNIF	mV	mVc	Lev	Lev-A
1000	0.187	0.003	0.020	0.016	0.024	0.031
1500	0.195	0.005	0.022	0.017	0.022	0.033
2000	0.193	0.007	0.021	0.018	0.026	0.036
2500	0.194	0.004	0.027	0.022	0.024	0.036

Table 4: Empirical MSE for Poisson regression demonstrated in Table 3. The numbers in the parentheses are the standard errors.

r	UNIF	MV	MVc	Lev	Lev-A
1000	0.0091 (0.0065)	0.0064 (0.0041)	0.0088 (0.0051)	0.0088 (0.0065)	0.0095 (0.0068)
1500	0.0071 (0.0054)	0.0047 (0.0034)	0.0049 (0.0038)	0.0067 (0.0049)	0.0070 (0.0051)
2000	0.0056 (0.0043)	0.0037 (0.0026)	0.0040 (0.0031)	0.0054 (0.0041)	0.0054 (0.0040)
2500	0.0045 (0.0032)	0.0030 (0.0021)	0.0033 (0.0025)	0.0044 (0.0034)	0.0047 (0.0036)

Table 5: Computing time (in second) for Poisson regression with $n = 100,000$, dimension $p = 80$, different values of r, and a fixed $r_0 = 400$.

r	FULL	UNIF	mV	mVc	Lev	Lev-A
1000	11.738	0.129	0.638	0.218	0.475	0.557
1500	11.659	0.163	0.689	0.253	0.514	0.595
2000	11.698	0.203	0.725	0.296	0.552	0.637
2500	12.005	0.240	0.777	0.339	0.602	0.681

Table 6: Empirical MSE for Poisson regression demonstrated in Table 5. The numbers in the parentheses are the standard errors.

r	UNIF	MV	MVc	Lev	Lev-A
1000	0.1003 (0.0174)	0.0786 (0.0135)	0.0782 (0.0136)	0.1011 (0.0172)	0.1021 (0.0192)
1500	0.0729 (0.0121)	0.0582 (0.0100)	0.0579 (0.0101)	0.0722 (0.0125)	0.0732 (0.0127)
2000	0.0562 (0.0095)	0.0472 (0.0085)	0.0470 (0.0085)	0.0565 (0.0094)	0.0577 (0.0099)
2500	0.0466 (0.0079)	0.0392 (0.0070)	0.0395 (0.0067)	0.0463 (0.0078)	0.0471 (0.0078)

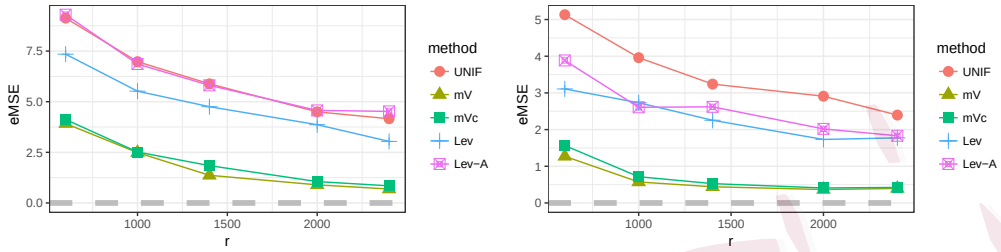
http://labrosa.ee.columbia.edu/millionsong/tasteprofile. One of the challenge of this dataset is to build a music recommendation system. As a basic step, it is interesting to predict the play counts by using the song information which has been collected in the Million Song Dataset (Bertin-Mahieux et al., 2011). Since the major mode and minor mode usually express different feelings, the play counts may perform differently under this two modes. Thus we only focus on major mode in this example. Besides the mode of music, the following six features are selected to describe the song characteristics: x_1, the duration of the track; x_2, the overall loudness of the song; x_3, tempo in BPM; x_4, artist hotttnesss; x_5, the song hotttnesss; x_6, the hottness of the album which is selected as the max value of the song hotttnesss in the album. Here, x_1, x_2 and x_3 are features of a specified song; x_4, x_5 and x_6 are features of the artist, audience and album respectively. The last three features are subjective assessments by The Echo Nest, and all of them are on a scale between 0 and 1. Since the first three variables in the data set are on different scales, we normalize them first. In addition, we drop the `NA` values in the dataset. After data cleaning, we have $n = 205,032$ data points. As a first attempt to capture the relationship between the play counts and all regressors described above, we fit the basic Poisson regression model and report the result in Figure 5a.

Another way of modeling count data is to use NBR. For comparison, we also report the results from NBR in Figure 5b with the size parameter select as $\theta = 1.4$ which indicates over-dispersion of the data.

Similar to the case of synthetic data sets, we also compare our method with uniform subsampling and the leverage score subsampling methods, and report the results for r varying from 600 to 2800. The empirical MSEs are reported in Figure 5. It is clear to that as r increase, the eMSE decreases quickly for all methods. Moreover, $\boldsymbol{\pi}^{\mathrm{mV}}$ and $\boldsymbol{\pi}^{\mathrm{mVc}}$ perform similarly, and are uniformly better than the uniform subsampling and leverage score subsampling for larger values of r. It also worth to mention that the MSE in negative binomial regression is less than the Poisson regression. This is because the ratio of square Winsorized mean and Winsorized variance of $\boldsymbol{y}$ is around 1.4 which implies the data is over-dispersed. This echoes the results in Theorem 5 which advise us to include more subsamples for worse goodness of fitting.

Supplementary Materials

Technical proofs and additional simulation results are included in the online supplementary material.



(a) Poisson Regression (b) Negative Binomial Regression

Figure 5: Empirical MSEs for different second step subsample size r with the first step subsample size being fixed at $r_0 = 400$.

Acknowledgement

The authors sincerely thank the editor, the associate editor and two referees for their valuable comments which led to significant improvement of the manuscript. The authors would like to thank Prof. Jinzhu Jia for his helpful suggestions and discussions. Ai'work is supported by NNSF of China grants 11671019 and LMEQF. Wang's work is partially supported by NSF grant 1812013 and an UConn REP grant.

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