Nearly optimal capture–recapture sampling and empirical likelihood weighting estimation for M-estimation with big data

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Abstract

Subsampling techniques can reduce the computational costs of processing big data. Practical subsampling plans typically involve initial uniform sampling and refined sampling. With a subsample, big data inferences are generally built on the inverse probability weighting (IPW), which becomes unstable when the probability weights are close to zero and cannot incorporate auxiliary information. First, we consider capture–recapture sampling, which combines an initial uniform sampling with a second Poisson sampling. Under this sampling plan, we propose an empirical likelihood weighting (ELW) estimation approach to an M-estimation parameter. Second, based on the ELW method, we construct a nearly optimal capture–recapture sampling plan that balances estimation efficiency and computational costs. Third, we derive methods for determining the smallest sample sizes with which the proposed sampling-and-estimation method produces estimators of guaranteed precision. Our ELW method overcomes the instability of IPW by circumventing the use of inverse probabilities, and utilizes auxiliary information including the size and certain sample moments of big data. We show that the proposed ELW method produces more efficient estimators than IPW, leading to more efficient optimal sampling plans and more economical sample sizes for a prespecified estimation precision. These advantages are confirmed through simulation studies and real data analyses.

Keywords: Big data; Capture–recapture sampling; Empirical likelihood; M-estimation; Sample size formula.

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1 Introduction

One of the most significant features of big data is its incredibly large volume, which poses serious challenges to its timely processing. Data analytics need to be performed efficiently so that the results are made available to users in a cost-effective and timely manner. A popular and efficient strategy for solving this problem is to draw small-scale subsamples from the big data (original sample) and make statistical inferences based on the subsamples (Drineas et al. 2006, 2011). Compared with the original big data, the subsamples are usually much smaller, and so subsample-based inferences significantly reduce the required computational resources.

Subsample-based inferences for big data generally involve two fundamental issues: how to draw an effective subsample and how to make efficient statistical inferences based on the subsample. Regarding the first issue, it is generally accepted that carefully designed sampling probabilities make unequal probability samplings more efficient than simple random or uniform sampling. Many researchers have developed efficient or optimal sampling plans for frequently encountered parametric statistical problems, including linear regression models (Ma et al. 2014), logistic regression (Fithian and Hastie 2014, Wang 2019), generalized linear models (Ai et al. 2022), quantile regression (Ai et al. 2021, Fan et al. 2021, Wang and Ma 2021), and more general models (Shen et al. 2021, Yu et al. 2022). All of the aforementioned methods use sampling with replacement, except those of Fithian and Hastie (2014), Wang (2019), Shen et al. (2021), and Yu et al. (2022), which consider Poisson sampling, one of the easiest-to-implement sampling without replacement systems. Under Poisson sampling, the samples are independently drawn according to Bernoulli experiments with prespecified success probabilities. Poisson sampling has two advantages over sampling with replacement: it never draws replicate observations and its implementation is free from
memory constraints (Yao and Wang, 2019).

For the second issue, subsample-based statistical inferences for big data are usually performed through inverse probability weighting (IPW), which leads to the Hansen–Hurwitz estimator (Hansen and Hurwitz, 1943) under sampling with replacement and to the Horvitz–Thompson estimator (Horvitz and Thompson, 1952) under sampling without replacement. However, the subsample-based IPW estimation procedure for big data analysis suffers from two weaknesses. First, the IPW estimator can be highly unstable if there are extremely small probabilities, resulting in poor finite-sample performance of the accompanying asymptotic-normality-based inferences (Kang and Schafer, 2007; Robins et al., 2007; Cao et al., 2009; Imbens and Wooldridge, 2009; Busso et al., 2014; Han et al., 2019). This weakness of the IPW estimator has been observed in survey sampling (Zong et al., 2019) and areas such as missing data problems (Robins et al., 2007), treatment effect estimation (Crump et al., 2009; Khan and Tamer, 2010; Yang and Ding, 2018), and survival analysis (Robins and Finkelstein, 2000; Dong et al., 2020). To circumvent this notorious issue, an unnatural lower boundedness assumption is often imposed on the probabilities (Rosenbaum and Rubin, 1983; McCaffrey et al., 2013; Sun and Tchetgen Tchetgen, 2018). However, tiny probabilities are frequently encountered in practice, especially when the propensity scores are estimated from data (Yang and Ding, 2018; Ma and Wang, 2020). Second, the efficiency of IPW cannot be enhanced by incorporating auxiliary information, although this is often available in big data analysis. For example, the sample mean of some variables in a big dataset can be quickly calculated at little computational cost; this can be taken as auxiliary information when inferences are made based on a subsample. To overcome the first limitation of IPW, Liu and Fan (2021) proposed a biased-sample empirical likelihood (EL) weighting method to serve the same general purpose as IPW, which completely overcomes
the instability of IPW-type estimators by circumventing the use of inverse probabilities. However, their EL method does not take into account the auxiliary information defined by general estimating equations.

In the case of big data, the optimal sampling depends on the statistical problem under study and the accompanying subsample-based estimation procedure. To consider both the generality and convenience of theoretical analysis and implementation, we focus on M-estimation problems with convex loss functions, and consider the use of Poisson sampling. Popular examples of M-estimation problems with convex loss functions include linear regression, quantile regression, and many generalized linear regressions (e.g., logistic regression, softmax regression, and Poisson regression). The sampling probabilities of the ideal optimal samplings depend on the ideal parameter estimator from the big data itself. For the optimal sampling to be practically applicable, an initial sample is required to produce an initial estimate of the parameter of interest. In this paper, we regard each of two samplings as a capture, and hence regard the whole sampling procedure as a capture–recapture sampling. This is a novel viewpoint in the study of subsampling for big data. Capture–recapture sampling is widely used to estimate population sizes in biology, ecology, and reliability studies [McCrea and Morgan 2014]. A significant difference between capture–recapture sampling for big data analysis and the equivalent methods for biology, ecology, and reliability studies is that the “population size” is known in the former, whereas it is unknown, and constitutes the target parameter to be estimated, in the latter.

This paper makes three contributions to the literature of subsample-based big data analysis.

1. First, we develop an empirical likelihood weighting (ELW) estimation method for a capture–recapture sample from big data, incorporating auxiliary information defined
by estimating equations. The proposed estimation procedure not only overcomes the
instability of the IPW by circumventing the use of inverse probabilities, but also
achieves enhanced efficiency by incorporating auxiliary information. We show that,
in theory, the proposed ELW estimator is asymptotically more efficient than the IPW
estimator.

2. Second, balancing the estimation efficiency with the computational costs, we con-
struct a nearly optimal capture–recapture sampling plan by minimizing the upper
bound of the asymptotic mean square error (MSE) of the proposed ELW estimator.
The sample from the first capture is used to estimate the subsampling probabilities
of the second capture.

3. Third, we determine the minimal sample size needed so that the proposed nearly
optimal sampling plan achieves the desired precision requirement in terms of MSE
and absolute error. As the ELW estimator is more efficient than the IPW estimator,
the proposed nearly optimal capture–recapture sampling is expected to outperform
existing optimal IPW-based subsampling plans.

The remainder of this paper is organized as follows. In Section 2 after introducing the
M-estimation problem and the commonly used IPW estimation method, we introduce the
ELW estimation procedure with auxiliary information under a general capture–recapture
sampling plan, and study the asymptotic behavior of the ELW estimator. In Section 3,
we construct a nearly optimal capture–recapture sampling plan and discuss its practical
implementation. In Section 4, we derive the minimal sample size needed for the proposed
estimator to meet a prespecified precision. Simulation studies and real applications are
reported in Sections 5 and 6. Finally, Section 7 concludes with a discussion. All technical
proofs are given in the supplementary material for clarity.
2 Empirical likelihood weighting estimation

2.1 Setup and IPW

Suppose that the big data consist of $N$ observations $\{Z_i\}_{i=1}^N$, which are independent and identically distributed (i.i.d.) copies from a population $Z$ with an unknown cumulative distribution function $F$. Parametric models indexed by a $q$-dimensional parameter $\theta$ are usually imposed to extract information from data. Let $\ell(z, \theta)$ be a user-specific convex loss function that quantifies the lack-of-fit of a parametric model indexed by a parameter $\theta$ based on an observation $z$. The average loss or risk function is $R(\theta) = \mathbb{E}\{\ell(Z, \theta)\} = \int \ell(z, \theta)dF(z)$. We define the parameter of interest $\theta_0$ to be the risk minimizer (Huber, 2011; Shen et al., 2021)

$$\theta_0 = \arg\min_{\theta} R(\theta).$$

This setup includes many common problems as special cases. When $Z$ is a scalar, the true parameter value $\theta_0$ is the mean or median of $Z$ if $\ell(Z, \theta) = (Z - \theta)^2$ or $|Z - \theta|$. When $Z = (Y, X^\top)^\top$, $\theta_0$ may be the population-level regression coefficient in the generalized linear regression, least-squares regression, quantile regression, and expectile regression models under the specification of $\ell(z; \theta)$ given in Table 1.

Based on the big-data observations, $\hat{\theta}_N = \arg\min_\theta \sum_{i=1}^N \ell(Z_i, \theta)$ is the ideal estimator of $\theta$. For massive datasets, $N$ can be so large that the direct calculation of $\hat{\theta}_N$ is formidable or practically infeasible. Subsampling techniques then come into play to reduce the computation costs. As discussed in the introduction, we consider the use of capture-recapture sampling, where the first capture is a Poisson sampling with an equal sampling probability and the second capture is another Poisson sampling, but with generally unequal sampling probabilities. Let the unequal sampling probabilities in the second capture be $\pi_i = \pi(Z_i)$,
Table 1: Loss functions and the matrix $V$ under commonly-used regression models. Here $\ddot{a}(x)$ is the second derivative of $a(x)$.

| Regression model | $\ell(z; \theta)$ | $V$ |
|------------------|--------------------|-----|
| Generalized linear | $-yx^\top + a(x^\top) - \log\{b(y)\}$ | $\mathbb{E}\{XX^\top \ddot{a}(X^\top \theta_0)\}$ |
| Poisson | $-yx^\top + \exp(x^\top \theta) + \log(y!)$ | $\mathbb{E}\{XX^\top \exp(X^\top \theta_0)\}$ |
| Logistic | $-yx^\top + \log\{1 + \exp(x^\top \theta)\}$ | $\mathbb{E}\left[XX^\top \frac{\exp(x^\top \theta_0)}{(1+\exp(x^\top \theta_0))^2}\right]$ |
| Least square | $(y - x^\top \theta)^2$ | $\mathbb{E}(XX^\top)$ |
| Quantile | $(y - x^\top \theta)\{\tau - I(y - x^\top \theta < 0)\}$ | $\mathbb{E}\{XX^\top f(X^\top \theta_0 | X)\}$ |
| Expectile | $(y - x^\top \theta)^2|\tau - I(y - x^\top \theta < 0)|$ | $\mathbb{E}\{XX^\top |\tau - I(Y \leq X^\top \theta_0)\}|$ |

$i = 1, \ldots, N$, for some function $\pi(\cdot)$. The ideal sample sizes for both the Poisson samplings in the capture–recapture sampling plan, $r_0$ and $r = \sum_{i=1}^N \pi_i$, must be specified beforehand.

In the first capture, for each $Z_i$ ($i = 1, 2, \ldots, N$), we conduct a Bernoulli experiment with success probability $\alpha_{10} = r_0/N$ and denote the result as $D_{i1}$, which is equal to 1 for success and 0 otherwise. Datum $Z_i$ is sampled in the first capture if and only if $D_{i1} = 1$. The samples in the first capture are used to produce an initial estimate of $\theta$, which is then employed to determine the sampling probabilities of the second capture. For now, we assume that the $\pi_i$ are known. In the second capture, we again conduct a Bernoulli experiment, but with success probability $\pi_i$ for datum $Z_i$, and denote the result as $D_{i2}$; in the second capture, datum $Z_i$ is sampled if and only if $D_{i2} = 1$. Finally, the resulting capture–recapture sample can be written as $\{(D_iZ_i, D_{i1}, D_{i2}), \; i = 1, 2, \ldots, N\}$, where $D_i = I(D_{i1} + D_{i2} > 0)$ and $I(\cdot)$ is the indicator function.

**Assumption 1** The $N$ random vectors $(Z_i, D_{i1}, D_{i2})$ ($i = 1, \ldots, N$) are i.i.d. copies of $(Z, D_{(1)}, D_{(2)})$. Suppose that the distribution $F(z)$ of $Z$ is nondegenerate, $\mathbb{E}(D_{(1)}|Z) =$
\[ E(D_{(1)}) = \alpha_{10}, \quad E(D_{(2)}|Z) = \pi(Z), \quad \text{and} \quad \alpha_{20} = E(D_{(2)}) = E\{\pi(Z)\}. \]

Let \( D = I(D_{(1)} + D_{(2)} > 0) \), where \( D_{(1)} \) and \( D_{(2)} \) are as defined in Assumption 1. Then, \( E(D) = 1 - (1 - E(D_{(1)}))\{1 - E(D_{(2)})\} = 1 - (1 - \alpha_{10})(1 - \alpha_{20}) \). For a given datum \( Z \), the overall probability of being sampled is \( \varphi(Z) = E(D \mid Z) = 1 - (1 - \alpha_{10})\{1 - \pi(Z)\} \) under Assumption 1. Based on the capture-recapture sample, the IPW estimator of \( \theta \) is

\[
\hat{\theta}_{\text{IPW}} = \arg \min_{\theta} \hat{R}_{\text{IPW}}(\theta) \equiv \arg \min_{\theta} \frac{1}{N} \sum_{i=1}^{N} \frac{D_i}{\varphi(Z_i)} \ell(Z_i, \theta), \tag{2}
\]

where \( \hat{R}_{\text{IPW}}(\theta) \) is the IPW estimator of the risk function \( R(\theta) \).

**Assumption 2** Suppose that \( \ell(z, \theta) \) is a loss function that is convex with respect to \( \theta \), and that \( \ell(z, \theta_0 + t) = \ell(z, \theta_0) + \ell(z)^\top t + \xi(z, t) \) holds in a neighborhood of \( t = 0 \). Here, \( \hat{\ell}(z) = \partial\ell(z, \theta_0)/\partial\theta \) satisfies \( \mathbb{E}\{\hat{\ell}(Z)\} = 0 \) and \( \mathbb{B}_{\ell\ell} = \mathbb{E}\{\hat{\ell}(Z)\hat{\ell}(Z)/\varphi(Z)\} \) is finite, and \( \xi(z, t) \) satisfies \( \mathbb{E}\{\xi(Z, t)\} = (1/2)t^\top V t + o(||t||^2) \) and \( \mathbb{E}\{\xi^2(Z, t)\} = o(||t||^2) \) for a positive-definite matrix \( V \) as \( ||t|| \to 0 \).

Assumption 2 is satisfied by many common regression models, such as those in Table 1, where the corresponding matrices \( V \) are also provided for convenience of applications.

**Theorem 1** Suppose that Assumptions 1 and 2 are satisfied and that \( \alpha_{10}, \alpha_{20} \in (0, 1) \) are fixed quantities. As \( N \) goes to infinity, \( \sqrt{N}(\hat{\theta}_{\text{IPW}} - \theta_0) \xrightarrow{d} \mathcal{N}(0, \Sigma_{\text{IPW}}) \), where \( \xrightarrow{d} \) denotes “converges in distribution to” and \( \Sigma_{\text{IPW}} = V^{-1} \mathbb{B}_{\ell\ell} V^{-1} \).

As discussed in the introduction, if some probabilities \( \varphi(Z_i) \) are too close to zero, \( \hat{R}_{\text{IPW}}(\theta) \) exhibits remarkable instability, making the resulting IPW estimator \( \hat{\theta}_{\text{IPW}} \) in (2) undesirably unstable. In the context of big data analysis, auxiliary information is often available. For example, the response mean of a big data sample can often be quickly calculated with little extra effort, and can be regarded as auxiliary information in subsample-based analysis. However, the estimation efficiency of the IPW method cannot be enhanced
by incorporating auxiliary information. Based on optimal estimating function theory (Goddambe, 1960), the score function derived from the complete-data likelihood is optimal in the class of inverse weighting estimating functions (Qin, 2017, Section 5.2). This motivates us to consider the full-likelihood-based inference approach under the capture-recapture sampling.

### 2.2 ELW estimation under capture-recapture sampling

Given the capture-recapture data \( \{(D_i, Z_i, D_{i1}, D_{i2}) \mid i = 1, 2, \ldots, N \} \), the full likelihood is

\[
\left( \begin{array}{c} N \\ n \end{array} \right) \prod_{i=1}^{N} \left[ \{ \varphi(Z_i) dF(Z_i) \}^{D_i} \cdot (1 - \alpha)^{1-D_i} \right],
\]

(3)

where \( \alpha = \mathbb{E}(D) = \int \varphi(z) dF(z) \) is the marginal probability of observing a value of \( Z \).

The true value of \( \alpha \) is \( \alpha_0 = 1 - (1 - \alpha_{10})(1 - \alpha_{20}) \) under Assumption [1]. Following Liu and Fan (2021), we use the empirical likelihood method (Owen, 1988, 2001) to handle \( F(z) \). Using the principle of the empirical likelihood, we model \( F(z) \) by a step function \( \sum_{i=1}^{N} p_i I(Z_i \leq z) \), where the \( p_i \) are positive and sum to one.

Then, the full log-likelihood becomes the empirical log-likelihood

\[
\sum_{i=1}^{N} [D_i \log(p_i) + D_i \log\{\varphi(Z_i)\} + (1 - D_i) \log(1 - \alpha)],
\]

(4)

where the feasible \( p_i \) satisfy \( p_i \geq 0, \sum_{i=1}^{N} p_i = 1 \), and

\[
\sum_{i=1}^{N} p_i \{\varphi(Z_i) - \alpha\} = 0.
\]

(5)

The previous equation follows from \( \alpha = \int \varphi(z) dF(z) \). The \( Z_i \) with \( D_i = 0 \) are not observed. Although appearing in the expression of the above likelihood, they do not actually contribute to the likelihood. The expression of the empirical log-likelihood implies that only those \( p_i \) with \( D_i = 1 \) make a contribution to the likelihood.
If we take $\alpha$ to be an unknown parameter, Liu and Fan (2021) showed that the maximum point of (4) under the constraints $p_i \geq 0, \sum_{i=1}^{N} p_i = 1,$ and (5) is always well defined if there are at least two different values in $\{\varphi(Z_i) : D_i = 1, i = 1, 2, \ldots, N\}$ (or, equivalently, $\{\pi(Z_i) : D_i = 1, i = 1, 2, \ldots, N\}$). Liu and Fan (2021) took the resulting $p_i$, say $\tilde{p}_i$, as the weights and proposed a biased-sample empirical likelihood weighting estimation method that serves the same purpose as IPW, but overcomes the problem of instability. Regardless of whether it is known or not, the parameter $\alpha$ is treated as an unknown quantity in their method. As a result, their weighting method is always well defined, as their focus was to develop a new weighting method that is insensitive to small inclusion probabilities.

Under the two Poisson samplings in the capture–recapture sampling, the true parameter values $\alpha_{10}$ and $\alpha_{20}$ need to be prespecified prior to their implementation, so that $\alpha_0 = 1 - (1 - \alpha_{10})(1 - \alpha_{20})$ is known a priori. Unlike Liu and Fan (2021), we make full use of this and other auxiliary information to improve the efficiency of the resulting point estimator of $\theta$. The feasible $p_i$ should satisfy

$$\sum_{i=1}^{N} p_i \{\varphi(Z_i) - \alpha_0\} = 0.$$  

(6)

In addition, for massive datasets, although solving the optimization problem $\min \sum_{i=1}^{N} \ell(Z_i, \theta)$ is complicated and time-consuming, the big data sample mean $\sum_{i=1}^{N} Z_i / N$ or other sample moments can be calculated relatively easily. This can be taken as auxiliary information when we make statistical inferences about the big data based on a subsample. Suppose that $\tilde{h} = (1/N) \sum_{i=1}^{N} h(Z_i)$ is available for some function $h$, which may be vector-valued. For convenience, we assume that $\mathbb{E}\{h(Z)\} = 0$ is known. In practice, we recommend replacing $h(Z)$ by $h(Z) - \tilde{h}$. This can be formulated as one more estimating equation:

$$\sum_{i=1}^{N} p_i h(Z_i) = 0.$$  

(7)
In summary, we recommend estimating the \( p_i \) by their maximum empirical likelihood estimator, which is the maximizer of the empirical log-likelihood (4) under the constraints \( p_i \geq 0, \sum_{i=1}^{N} p_i = 1 \) and (6), (7). No nondegenerate solution to this optimization problem exists if the constraints do not hold simultaneously (Chen et al. 2008; Liu and Chen 2010), or, equivalently, if the origin lies outside of the convex hull of \( \{ h_e(Z_i) : D_i = 1, 1 \leq i \leq N \} \), where \( h_e(Z) = (\varphi(Z) - \alpha_0, h^\top(Z)) \). In this situation, the optimal weights \( \hat{p}_i \) are undefined, and we define them to be \( \tilde{p}_i \), which are the maximizers of (4) under the constraints \( p_i \geq 0, \sum_{i=1}^{N} p_i = 1 \) in the case of unknown \( \alpha \); see Liu and Fan (2021). Otherwise, by the Lagrange multiplier method, we have

\[
\hat{p}_i = \frac{1}{\sum_{j=1}^{N} D_j} \cdot \frac{D_i}{1 + \hat{\lambda}^\top h_e(Z_i)},
\]

where \( \hat{\lambda} \) is the solution to \( \sum_{i=1}^{N} D_i h_e(Z_i) / \{1 + \hat{\lambda}^\top h_e(Z_i)\} = 0 \).

Given \( \hat{p}_i \), we propose to estimate \( \theta \) by the ELW estimator

\[
\hat{\theta}_{ELW} = \arg \min_{\theta} \hat{R}_{ELW}(\theta) \equiv \arg \min_{\theta} \sum_{i=1}^{N} \hat{p}_i \ell(Z_i, \theta)
\]

where \( \hat{R}_{ELW}(\theta) \) is the ELW estimator of the risk function \( R(\theta) \). If the loss function \( \ell(z, \theta) \) is differentiable with respect to \( \theta \) for almost all \( z \), an alternative ELW estimator of \( \theta \) can be obtained by maximizing the empirical log-likelihood (4) under the constraints \( p_i \geq 0, \sum_{i=1}^{N} p_i = 1 \) with (6), (7), and \( \sum_{i=1}^{N} p_i \partial \ell(Z_i, \theta) / \partial \theta = 0 \). Because the dimensions of \( \theta \) and \( \partial \ell(Z_i, \theta) / \partial \theta \) are the same, the resulting maximum EL estimator is exactly equal to \( \hat{\theta}_{ELW} \).

**Theorem 2** Suppose that Assumptions [1] and [2] hold, \( B_{hh} = \mathbb{E}\{h_e(Z)h_e^\top(Z) / \varphi(Z)\} \) is positive-definite, and \( \alpha_{10}, \alpha_{20} \in (0, 1) \) are fixed and known. As \( N \) goes to infinity,

(a) \( \hat{\theta}_{ELW} \) is consistent with \( \theta_0 \) and \( \sqrt{N}(\hat{\theta}_{ELW} - \theta_0) = -V^{-1} \cdot N^{1/2} \sum_{i=1}^{N} \hat{p}_i \hat{\ell}(Z_i) + o_p(1) \);

(b) \( \sqrt{N}(\hat{\theta}_{ELW} - \theta_0) \xrightarrow{d} \mathcal{N}(0, \Sigma_{ELW}) \) with \( \Sigma_{ELW} = V^{-1}(B_{\hat{\ell}\hat{\ell}} - B_{\hat{\ell}h}B_{hh}^{-1}B_{h\hat{\ell}}^\top) V^{-1} \), where \( B_{\hat{\ell}h} = \mathbb{E}\{\hat{\ell}(Z)h_e^\top(Z) / \varphi(Z)\} \) and \( B_{\hat{\ell}\hat{\ell}} = \mathbb{E}\{\hat{\ell}(Z)\hat{\ell}^\top(Z) / \varphi(Z)\} \).
(c) If the auxiliary information defined by (7) is ignored, then \( \sqrt{N}(\hat{\theta}_{\text{ELW}} - \theta_0) \xrightarrow{d} \mathcal{N}(0, \Sigma_{\text{ELW}0}) \), where \( \Sigma_{\text{ELW}0} = V^{-1}\{B_{\ell\ell} - (B_{\ell\ell}B_{\ell\ell}^\top)/(B_{11} - \alpha_0^{-1})\}V^{-1} \) and \( B_{\ell\ell} = \mathbb{E}\{\ell(Z)/\varphi(Z)\} \).

Because \( \Sigma_{\text{IPW}} - \Sigma_{\text{ELW}} = V^{-1}B_{\ell h}B_{h h}^{-1}B_{h \ell}^\top V^{-1} \) is a nonnegative-definite matrix, the ELW estimator is asymptotically more efficient than the IPW estimator. This finding remains true even if we ignore constraint (7), or if no auxiliary information is incorporated in the ELW estimator. It can also be verified that \( \Sigma_{\text{ELW}0} - \Sigma_{\text{ELW}} = V^{-1}\{B_{\ell h}B_{h h}^{-1}B_{h \ell}^\top - (B_{\ell\ell}B_{\ell\ell}^\top)/(B_{11} - \alpha_0^{-1})\}V^{-1} \) is nonnegative-definite, which means that incorporating auxiliary information enhances the efficiency of the proposed ELW estimator.

### 2.3 Case with negligible sampling fraction

Thus far, we have assumed that the overall sampling fraction of the big data is nonnegligible, i.e. \( \alpha_0 \in (0, 1) \). When the volume of the big data is huge, it is reasonable to assume that the sampling fraction may be negligible.

**Assumption 3** Suppose there exist a positive sequence \( \{b_N\}_{N=1}^{\infty} \), a positive function \( 0 < \pi_*(Z) \leq 1 \), and a positive constant \( \alpha_{1*} \) such that \( b_N \to \infty \), \( b_N/N \to 0 \), \( b_N\pi(Z) \to \pi_*(Z) \), and \( b_N\alpha_{10} \to \alpha_{1*} \) as \( N \to \infty \).

Under Assumption 3 we have \( b_N\alpha_{20} = \mathbb{E}\{b_N\pi(Z)\} \to \alpha_{2*} = \mathbb{E}\{\pi_*(Z)\} \) as \( N \to \infty \). Define \( \alpha_0 = b_N\alpha_{10} + b_N\alpha_{20} \) and \( \varphi(Z) = b_N\alpha_{10} + b_N\pi(Z) \). Then, \( \alpha_0 \) and \( \varphi(Z) \) converge to \( \alpha_* = \alpha_{1*} + \alpha_{2*} \) and \( \varphi_*(Z) = \alpha_{1*} + \pi_*(Z) \), respectively. Because \( \alpha_{10} \) and the \( \pi(Z_i) \) are prespecified, the log-likelihood (4) under Assumption 3 up to a constant not depending on the unknown parameters \( p_i \), is equal to \( \sum_{i=1}^{N} D_i \log(p_i) \). Besides the constraints \( p_i \geq 0 \) and \( \sum_{i=1}^{N} p_i = 1 \), the \( p_i \) in this situation should satisfy \( \sum_{i=1}^{N} p_i h_{e*}(Z_i) = 0 \), where \( h_{e*}(Z) = (\varphi_*(Z) - \alpha_*, h^\top(Z))^\top \).
The maximum EL estimator of $p_i$ is $\hat{p}_i^* = n^{-1} \{1 + \tilde{\lambda}^\top h_{e^*}(Z_i)\}$, where $\tilde{\lambda}$ is the solution to

$$\frac{1}{n} \sum_{i=1}^{n} \frac{h_{e^*}(Z_i)}{1 + \tilde{\lambda}^\top h_{e^*}(Z_i)} = 0. \quad (10)$$

Our ELW estimator of $\theta$ is $\hat{\theta}_{ELW} = \arg \min_{\theta} \sum_{i=1}^{n} \hat{p}_i^* \ell(Z_i, \theta)$.

Theorem 3 Suppose that Assumptions 1–3 hold, the distribution of $Z$ is nondegenerate, and that $C_{hh^*} = \mathbb{E}\{h_{e^*}(Z)h_{e^*}(Z)/\varphi_*(Z)\}$ is positive-definite. As $N$ goes to infinity, $\sqrt{N/b_N}(\hat{\theta}_{ELW} - \theta_0) \xrightarrow{d} \mathcal{N}(0, \Sigma_{ELW^*})$ and $\sqrt{N/b_N}(\hat{\theta}_{IPW} - \theta_0) \xrightarrow{d} \mathcal{N}(0, \Sigma_{IPW^*})$, where

$$\Sigma_{ELW^*} = V^{-1}(C_{\ell\ell^*} - C_{\ell h^*}C_{hh^*}C_{\ell h^*})V^{-1} \quad \text{and} \quad \Sigma_{IPW^*} = V^{-1}C_{\ell\ell^*}V^{-1}$$

with $C_{\ell h^*} = \mathbb{E}\{\hat{\ell}(Z)h_{e^*}(Z)/\varphi_*(Z)\}$ and $C_{\ell\ell^*} = \mathbb{E}\{\hat{\ell}(Z)\hat{\ell}^\top(Z)/\varphi_*(Z)\}$.

Theorem 3 indicates that even as the sampling fraction tends to zero, both the ELW and IPW estimators are consistent at the rate $\sqrt{N/b_N}$, a lower rate than $\sqrt{N}$, and our ELW estimator is still asymptotically more efficient than the IPW estimator. Although the asymptotic results here are slightly different from those in Theorems 1 and 2, the variances of $\hat{\theta}_{ELW}$ and $\hat{\theta}_{IPW}$ can always be approximated by $\Sigma_{ELW}/N$ and $\Sigma_{IPW}/N$, respectively.

3 Optimal capture–recapture sampling plan

The asymptotic efficiency of subsample-based statistical inferences depends critically on the underlying subsampling plan. Carefully chosen sampling plans can lead to remarkable efficiency gains over uniform sampling, which motivates optimal subsampling for big data.

3.1 Ideal optimal sampling plan

MSE is a popular evaluation criterion for the performance of a point estimator. For a constant matrix $Q$, Theorem 2 implies that $N$ times the MSE of $Q\hat{\theta}_{ELW}$ is approximated
Because practical convenience. However, by respectively. When \( Q = V \), the MSE criterion is independent of \( V \), and hence has much practical convenience. However, \( Q = I \) is preferred when we are more interested in the efficiency of the ELW estimator itself.

Recall that

\[
B_{\hat{\ell}\hat{\ell}} = \mathbb{E} \left[ \frac{\hat{\ell}(Z, \theta_0) \hat{\ell}(Z, \theta_0)}{\varphi(Z)} \right], \quad B_{\hat{\ell}h} = \mathbb{E} \left\{ \frac{\hat{\ell}(Z, \theta_0) h_e^\top(Z)}{\varphi(Z)} \right\}, \quad B_{hh} = \mathbb{E} \left[ \frac{h_e(Z) \circ \circ}{\varphi(Z)} \right].
\]

Because \( h_e(Z) = (\varphi(Z) - \alpha_0, h^\top(Z)) \), \( \mathbb{E}\{\hat{\ell}(Z, \theta_0)\} = 0 \), and \( \mathbb{E}\{h(Z)\} = 0 \), we have

\[
B_{\hat{\ell}h} = \mathbb{E} \left\{ \frac{\hat{\ell}(Z, \theta_0)(-\alpha_0, h^\top(Z))}{\varphi(Z)} \right\}, \quad B_{hh} = \mathbb{E} \left[ \frac{(-\alpha_0, h^\top(Z))^\circ \circ}{\varphi(Z)} \right] - \alpha_0 e_1 \circ \circ,
\]

where \( e_1 \) is a unit vector in which the first component is 1. Let \( \pi = (\pi_1, \ldots, \pi_N) \) with \( \pi_i = \pi(Z_i) \), and \( \varphi = (\varphi_1, \ldots, \varphi_N) \), where \( \varphi_i = 1 - (1 - \alpha_{10})(1 - \pi_i) \). Given the sampling plan \( \pi \), natural consistent “estimators” of \( B_{\hat{\ell}\hat{\ell}}, B_{\hat{\ell}h}, \) and \( B_{hh} \) are

\[
\hat{B}_{\hat{\ell}\hat{\ell}} = \frac{1}{N} \sum_{i=1}^{N} \frac{\hat{\ell}(Z_i, \theta_0) \hat{\ell}(Z_i, \theta_0)}{\varphi_i}, \quad \hat{B}_{\hat{\ell}h} = \frac{1}{N} \sum_{i=1}^{N} \frac{\hat{\ell}(Z_i, \theta_0) b_i^\top}{\varphi_i}, \quad \hat{B}_{hh} = \frac{1}{N} \sum_{i=1}^{N} b_i \circ \circ - \alpha_0 e_1 \circ \circ,
\]

where \( b_i = (-\alpha_0, h^\top(Z_i))^\top \) for \( i = 1, \ldots, N \). Accordingly, a natural consistent “estimator” of \( N \times \text{Mse}(\hat{\theta}_{\text{ELW}}) \) is

\[
H_s(\varphi) = \text{tr}\left\{ QV^{-1}(\hat{B}_{\hat{\ell}\hat{\ell}} - \hat{B}_{\hat{\ell}h}\hat{B}_{hh}^{-1}\hat{B}_{\hat{\ell}h}^\top)V^{-1}Q^\top \right\}
\]

\[
= \frac{1}{N} \sum_{i=1}^{N} \|a_i(\theta_0)\|^2 \varphi_i^{-1} - \frac{1}{N} \text{tr} \left\{ \left( \sum_{i=1}^{N} \varphi_i^{-1} a_i(\theta_0) b_i^\top \right) \times \left( \sum_{i=1}^{N} (\varphi_i^{-1} b_i b_i^\top - \alpha_0 e_1 \circ \circ) \right)^{-1} \left( \sum_{i=1}^{N} \varphi_i^{-1} a_i(\theta_0) \right) \right\},
\]

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where \( a_i(\theta_0) = QV^{-1}\dot{\ell}(Z_i, \theta_0) \). Because there is a one-to-one map from \( \pi \) to \( \varphi \), determining the optimal sampling plan \( \pi \) is equivalent to determining the optimal \( \varphi \). The optimal \( \varphi \) in terms of parameter estimation accuracy is the solution to

\[
\min_{\varphi} H_*(\varphi) \quad \text{s.t.} \quad \sum_{i=1}^{N} \varphi_i = N\alpha_0, \quad \alpha_{10} < \varphi_i < 1 \quad \text{for} \quad i = 1, \ldots, N. \tag{11}
\]

Unfortunately, there is no closed-form solution to problem (11), which makes it impractical and motivates us to derive a nearly optimal sampling plan.

### 3.2 Nearly optimal sampling plan

Nearly optimal solutions to (11) can be obtained using several techniques. First, we replace the objective function \( H_*(\varphi) \) by \( H(\varphi) \), where

\[
H(\varphi) = \frac{1}{N} \sum_{i=1}^{N} \frac{\| a_i(\theta_0) \|^2}{\varphi_i} - \frac{1}{N} \text{tr} \left\{ \left( \sum_{i=1}^{N} a_i(\theta_0)b_i^T \right) \left( \sum_{i=1}^{N} b_i b_i^T \right)^{-1} \left( \sum_{i=1}^{N} b_i a_i^T(\theta_0) \right) \right\}.
\]

The fact that \( H_*(\varphi) \leq H(\varphi) \) holds for any \( \varphi \) implies that a sampling plan with a small \( H(\varphi) \) somehow leads to a small \( H_*(\varphi) \).

Second, we transform the constrained optimization problem (11) by substituting \( H(\varphi) \) for \( H_*(\varphi) \). Define

\[
H_1(\varphi, K) = \frac{1}{N} \sum_{i=1}^{N} \frac{\| a_i(\theta_0) - Kb_i \|^2}{\varphi_i},
\]

where \( K \) is a matrix of the same dimensions as \( a_i(\theta_0)b_i^T \). Because \( H_1(\varphi, K) \) is a convex function of \( (\varphi, K) \), it follows that

\[
\min_{\varphi} H(\varphi) = \min_{\varphi} \min_{K} H_1(\varphi, K) = \min_{\varphi, K} H_1(\varphi, K),
\]

and that the solution to (11) can be approximated by solving

\[
\min_{\varphi, K} H_1(\varphi, K) \quad \text{s.t.} \quad \sum_{i=1}^{N} \varphi_i = N\alpha_0, \quad \alpha_{10} < \varphi_i < 1 \quad \text{for} \quad i = 1, \ldots, N. \tag{12}
\]
If we discard the inequality constraints and retain the equality constraint, then

$$\min_{\varphi, K} H_1(\varphi, K) = \min_K \{ \min_\varphi H_1(\varphi, K) \} = \min_K \frac{H_2(K)^2}{N^2 \alpha_0} = \frac{\{ \min_K H_2(K) \}^2}{N^2 \alpha_0},$$

where $H_2(K) = \sum_{i=1}^N \| a_i(\theta_0) - K b_i \|$. Denote $\hat{K} = \arg \min_K H_2(K)$. In this situation, a nearly optimal $\varphi$ is $\hat{\varphi} = (\hat{\varphi}_1, \ldots, \hat{\varphi}_N)$ with

$$\hat{\varphi}_i = \alpha_0 \cdot \frac{\| a_i(\theta_0) - \hat{K} b_i \|}{N - 1 \sum_{j=1}^N \| a_j(\theta_0) - \hat{K} b_j \|}. \quad (13)$$

Note that $\hat{\varphi}$ is generally different from $\hat{\varphi}^* = (\hat{\varphi}_1^*, \ldots, \hat{\varphi}_N^*)$, which is the minimizer of problem (12), because the optimization problems with and without the inequality constraint $\alpha_{10} < \varphi_i < 1$ ($i = 1, \ldots, N$) are not equivalent. From a practical perspective, we propose to take $\hat{K}$ as an approximation of $\hat{K}^*$ and adopt the optimal sampling plan with $\varphi$ solving

$$\min_{\varphi} H_1(\varphi, \hat{K}) \quad \text{s.t.} \quad \sum_{i=1}^N \varphi_i = N \alpha_0, \ \alpha_{10} < \varphi_i < 1 \text{ for } i = 1, \ldots, N. \quad (14)$$

By the Karush–Kuhn–Tucker condition, the solution to (14) is

$$\hat{\varphi}_{ei} = \max \left\{ \alpha_{10}, \ \min \left( \hat{\gamma} \cdot \frac{\| a_i(\theta_0) - \hat{K} b_i \|}{N - 1 \sum_{j=1}^N \| a_j(\theta_0) - \hat{K} b_j \|}, 1 \right) \right\}, \quad (15)$$

where the subscript “e” denotes that $\hat{\varphi}_{ei}$ is the “exact” solution to (14), and $\hat{\gamma} > 0$ is the solution to

$$N^{-1} \sum_{i=1}^N \max \left\{ \alpha_{10}, \ \min \left( \gamma \cdot \frac{\| a_i(\theta_0) - \hat{K} b_i \|}{N - 1 \sum_{j=1}^N \| a_j(\theta_0) - \hat{K} b_j \|}, 1 \right) \right\} = \alpha_0.$$

### 3.3 Practical considerations

The sampling plans with $\hat{\varphi}_i$ and $\hat{\varphi}_{ei}$ are not practically applicable, because both of them depend on $\theta_0$, which needs to be estimated beforehand. To this end, the convention is to draw an initial sample, say $\{ \tilde{z}_i = (\tilde{y}_i, \tilde{x}_i^\top) : i = 1, \ldots, m \}$, by uniformly sampling from the big data being studied. The first capture in our capture–recapture sampling plays
exactly the same role. Let \( \hat{\theta}_m = \arg \min_{\theta} \sum_{i=1}^{m} \ell(\tilde{z}_i, \theta) \) and \( \tilde{V} \) be a consistent estimator of \( V \) based on the first-capture sample. Denote \( \tilde{K} = \arg \min \sum_{i=1}^{m} \|\tilde{a}_i - \tilde{K}\tilde{b}_i\| \), where \( \tilde{b}_i = (-\alpha_0, h^\top(\tilde{z}_i))^\top \), and \( \tilde{a}_i = \tilde{V}^{-1}\ell(\tilde{z}_i, \tilde{\theta}_m) \) in the A-criterion or \( \tilde{a}_i = \ell(\tilde{z}_i, \tilde{\theta}_m) \) in the L-criterion. Calculating \( \tilde{K} \) may be computationally intensive, and so we use the least-squares estimate \( \hat{\tilde{K}} = \left( \sum_{k=1}^{m} \tilde{a}_k \tilde{b}_k^\top \right) \left( \sum_{j=1}^{m} \tilde{b}_j \tilde{b}_j^\top \right)^{-1} \) instead. Define

\[
\hat{\varphi}_{ei} = \max \left\{ \alpha_{10}, \min \left( \tilde{\gamma} \cdot \frac{\|\tilde{a}_i - \tilde{K}\tilde{b}_i\|}{m^{-1} \sum_{j=1}^{m} \|\tilde{a}_j - \tilde{K}\tilde{b}_j\|}, 1 \right) \right\},
\]

(16)

where \( \tilde{\gamma} > 0 \) is the smallest solution to

\[
m^{-1} \sum_{i=1}^{m} \max \left\{ \alpha_{10}, \min \left( \gamma \cdot \frac{\|\tilde{a}_i - \tilde{K}\tilde{b}_i\|}{m^{-1} \sum_{j=1}^{m} \|\tilde{a}_j - \tilde{K}\tilde{b}_j\|}, 1 \right) \right\} = \alpha_{10}.
\]

Our recommended sampling plan for the second capture is \( \tilde{\pi} = (\tilde{\pi}_1, \ldots, \tilde{\pi}_N) \) with \( \tilde{\pi}_i = (\hat{\varphi}_{ei} - \alpha_{10})/(1 - \alpha_{10}) \), where \( \alpha_{10} \in (0, 1) \) is the known sampling fraction of the first capture.

For the models in Table 1 (except the quantile regression model), the matrix \( V \) can be consistently estimated by the moment estimation method based on the first-capture sample. The estimation of \( V \) in the quantile regression model is more challenging because it depends on the unknown conditional density function \( f(y \mid x) \). Following Powell (1990), we estimate this \( V \) using the kernel estimator \( \hat{V} = (mh_m)^{-1} \sum_{i=1}^{m} K\{ (\hat{y}_i - \hat{x}_i^\top \hat{\theta}_m)/h_m \} \hat{x}_i \hat{x}_i^\top \), where \( K(\cdot) \) is a kernel function, usually chosen to be a density function, and \( h_m \) is the bandwidth.

### 4 Sample size determination

For a given subsample, the performance of the IPW and ELW estimators depends not only on the underlying sampling plan, but also on the size of the subsample. If the size \( n \) or the ideal size \( n_0 \) of a Poisson subsample is too small, the resulting estimator will be so unstable that it does not make any sense. When the (optimal) sampling plan is fixed,
it is necessary to specify the subsample size that guarantees the resulting estimate meets a certain precision requirement. To the best of our knowledge, this issue has never been discussed in the literature of subsampling for big data. We address the issue of determining \( n_0 \) under two precision requirements on \( \hat{\theta}_{ELW} \): (R1) The MSE of \( \hat{\theta}_{ELW} \) is no greater than a prespecified positive constant \( C_0 \), i.e., \( \text{Mse}(\hat{\theta}_{ELW}) \leq C_0 \). (R2) The absolute error of \( \hat{\theta}_{ELW} \) is no greater than a critical value \( d > 0 \) at the confidence level \( (1 - a) \), i.e.,

\[
P(\|\hat{\theta}_{ELW} - \theta_0\| \leq d) \geq 1 - a.
\]

(17)

We assume that the sample fraction \( \alpha_{10} > 0 \) of the first capture is known, but that for the second capture \( \alpha_{20} \) is unknown. Because \( n_0/N = \alpha_0 = 1 - (1 - \alpha_{10})(1 - \alpha_{20}) \), when the (optimal) sampling plan is fixed, determining \( \alpha_{20} \) is equivalent to determining \( n_0 \). Recall that a nearly optimal subsampling plan can be approximated by (13) or \( \tilde{\phi}_* = (\tilde{\phi}_{s1}, \ldots, \tilde{\phi}_{sN}) \), where \( \tilde{\phi}_{si} \) is \( \hat{\phi}_i \) with \( \hat{K} \) replaced by \( \tilde{K} \). With the sampling plan \( \tilde{\phi}_* \), an upper bound for the MSE of \( \hat{\theta}_{ELW} \) is

\[
H(\tilde{\phi}_*)/N = \frac{1}{N^3\alpha_0} \left\{ \sum_{j=1}^N \|a_j(\theta_0) - \tilde{K}\tilde{b}_j\| \right\}^2 = \frac{1}{n_0} \left\{ \frac{1}{N} \sum_{j=1}^N \|a_j(\theta_0) - \tilde{K}\tilde{b}_j\| \right\}^2,
\]

which can be estimated by \( n_0^{-1}\{m^{-1}\sum_{j=1}^m \|\tilde{a}_j - \tilde{K}\tilde{b}_j\|\}^2 \). Under requirement (R1), a sufficient approximation is to constrain \( n_0^{-1}\{m^{-1}\sum_{j=1}^m \|\tilde{a}_j - \tilde{K}\tilde{b}_j\|\}^2 \leq C_0 \). Note that the elements of \( \tilde{K} \) and \( \tilde{b}_j \) contain the unknown parameter \( \alpha_0 = n_0/N \). Therefore, the minimal sample size \( n_0 \) that satisfies requirement (R1) should be the solution to

\[
n_0 = \frac{1}{C_0} \left\{ \frac{1}{m} \sum_{j=1}^m \|\tilde{a}_j - \tilde{K}\tilde{b}_j\| \right\}^2.
\]

(18)

This is our first recommended sample size determination method, which we denote as M1 for convenience.

To determine the sample size under requirement (R2), note that the inequality \( \|\hat{\theta}_{ELW} - \theta_0\| \leq d \) is equivalent to \( \zeta^\top \Sigma_{ELW} \zeta \leq Nd^2 \), where \( \zeta = \sqrt{N} \Sigma^{-1/2}_{ELW}(\hat{\theta}_{ELW} - \theta_0) \) approximately
follows the $q$-dimensional standard normal distribution, where $q$ is the dimension of $\theta$. The distribution of $\zeta^\top \Sigma_{\text{ELW}} \zeta$ can be further approximated by a weighted chi-square distribution of $\sum_{k=1}^{q} \lambda_k \zeta_k^2$, where the $\lambda_k$ are the eigenvalues of $\Sigma_{\text{ELW}}$ and the $\zeta_k$ are i.i.d. standard normal random variables. According to Kim et al. (2006) [Lemma 2, page 453], the cumulative distribution of $\sum_{k=1}^{p} \lambda_k \zeta_k^2$ can be approximated by that of $\nu \chi^2_{\nu}$, where $\nu = \sum_{k=1}^{q} \lambda_k / \sum_{j=1}^{q} \lambda_j^2$. It follows that $P(\|\hat{\theta}_{\text{ELW}} - \theta_0\| \leq d) \approx P(\chi^2_{\nu} \leq \nu N d^2)$, which together with (17) implies the approximation $\nu N d^2 = \chi^2_{\nu}(1 - a)$, where $\chi^2_{\nu}(1 - a)$ is the $(1 - a)$th quantile of the chi-square distribution with $\nu$ degrees of freedom.

Moreover, $\nu$ is approximately equal to $\tilde{\nu} = \sum_{k=1}^{q} \tilde{\lambda}_k / \sum_{j=1}^{q} \tilde{\lambda}_j^2$, where the $\tilde{\lambda}_k$ are the eigenvalues of $\tilde{\Sigma}_{\text{ELW}} = \tilde{V}^{-1}(\tilde{B}_{\ell\ell} - \tilde{B}_{\ell h} \tilde{B}_{h h}^{-1} \tilde{B}_{h h}^\top) \tilde{V}^{-1}$. Herein, $\tilde{B}_{\ell\ell}$, $\tilde{B}_{\ell h}$, and $\tilde{B}_{h h}$ are the sample-mean estimates of $B_{\ell\ell}$, $B_{\ell h}$, and $B_{h h}$ based on the first-capture sample. Because $\Sigma_{\text{ELW}}$ (and hence $\lambda_k$) depends on $\alpha_0 = n_0 / N$, so do $\tilde{\Sigma}_{\text{ELW}}$, $\tilde{\lambda}_k$, and $\tilde{\nu}$. We denote $\tilde{\nu}$ by $\tilde{\nu}(n_0)$ to highlight this dependence. Our recommended sample size $n_0$ under requirement (R2), denoted as $M2$, is the root of

$$
\tilde{\nu}(n_0) = \nu_*,
$$

where $\nu_*$ is the solution to $\nu N d^2 = \chi^2_{\nu}(1 - a)$ with respect to $\nu$.

## 5 Simulations

In this section, we present the results of simulations to evaluate the finite-sample performance of the proposed estimation and sampling strategy and the sample size determination method.
5.1 Simulation settings

We generate a big dataset of size $N = 50,000$ from each of the following three examples, corresponding to Poisson regression, binomial regression, and quantile regression models.

**Example 1 (Poisson regression)** Given $X, Y$ follows a Poisson regression model with $\mathbb{E}(Y|X) = \exp(X^\top \theta_0)$ and $\theta_0 = -0.5 \times (1, 1, 1, 1, 1, 1, 1)^\top$. Four scenarios are considered to generate the covariates $X_i = (X_{i1}, \ldots, X_{i7})^\top$: Case 1. $X_{ij}$ are i.i.d. from $U(0,1)$, the standard uniform distribution; Case 2. $X_{ij}$ for $j \neq 2$ and $\varepsilon_i$ are i.i.d. from $U(0,1)$, and take $X_{i2} = X_{i1} + \varepsilon_i$. In this case, the correlation coefficient of $X_{i1}$ and $X_{i2}$ is around 0.7. Case 3. The same setting as case 2, except that $\varepsilon_i \sim U(0,0.1)$. In this case, the correlation coefficient of $X_{i1}$ and $X_{i2}$ is around 0.995. Case 4. The same setting as case 2, except that $X_{i6}$ and $X_{i7}$ are i.i.d. from $U(-1,1)$. In this case, the covariates have different supports.

**Example 2 (Logistic regression)** The settings here are the same as those in Example 1, except that $Y$ given $X$ follows a logistic regression model with mean $\mathbb{E}(Y|X) = \exp(\theta_0^\top X)/(1 + \exp(\theta_0^\top X))$.

**Example 3 (Quantile regression)** Given $X, Y$ follows a linear regression model $Y = \beta_0^\top X + \epsilon$, where $X = (1, X_2, \ldots, X_5)^\top$, $X_2, \ldots, X_5$ are i.i.d. from $N(0,1)$, $\beta_0 = -0.5 \times (1, 1, 1, 1, 1)^\top$, and the error distribution is to be specified. Given $\tau \in (0,1)$, $Q_\tau(Y|X) = \beta_0^\top X + Q_\tau(\epsilon)$, where $Q_\tau(\epsilon)$ is the $\tau$th quantile of $\epsilon$, and $\theta_0 = (Q_\tau(\epsilon)-0.5, -0.5, -0.5, -0.5, -0.5)^\top$.

We consider four combinations of error distribution and $\tau$: Case 1. $N(0,1)$ and $\tau = 0.5$; Case 2. $N(0,1)$ and $\tau = 0.75$; Case 3. $|N(0,1)|$ and $\tau = 0.5$; Case 4. $|N(0,1)|$ and $\tau = 0.75$.

We take the response mean of the big data as auxiliary information. Let ELW and ELWAI denote the ELW methods without and with the auxiliary information, together
with the corresponding nearly optimal capture–recapture sampling plan. We compare
the performance of ELW and ELWAI with UNIF, the usual M-estimation with one-step
uniform sampling, and the IPW method together with the corresponding optimal sampling
plan. In Examples 1 and 2, the MV subsampling probabilities of Yu et al. (2022) are
used in IPW, while in Example 3, IPW is chosen to be the OSQR of Fan et al. (2021),
which is also an IPW-based method. Note that a shrinkage technique was used with a
tuning parameter $\varrho$ when calculating the MV optimal subsampling probabilities in Yu
et al. (2022) [equation (21)]. For consistency with the setup of Yu et al. (2022), we fix $\varrho = 0.2$
in our numerical studies. If an initial sample (the first capture) is required for a method,
we fix its average sample size $r_0$ to be 200. We consider the average size $r$ of the second
sample (the recapture) to be 300, 500, 700, 1000, 1200, 1500, 1700, and 2000, respectively.
To ensure a fair comparison, we set the average sample size to $r_0 + r$ for UNIF.

5.2 Comparison of estimation efficiency

Under the A- and L-criteria, we generate 5000 subsamples by each of the methods under
comparison in each scenario of Examples 1–3. We compare the performance of the methods
in terms of the empirical MSE

$$MSE = \frac{1}{5000} \sum_{b=1}^{5000} \|\hat{\theta}_b - \hat{\theta}_N\|^2,$$

(20)

where $\hat{\theta}_b$ is a generic estimate in the $b$th repetition and $\hat{\theta}_N$ is the M-estimator based on the
big data. Figures 1 and 2 display the logarithms of empirical MSE versus $r$ under the A-
and L-criteria, respectively.

We first examine the results in Figure 1 under the A-criterion. In this case, the empirical
MSEs in (20) are good approximations for the asymptotic MSEs of the four estimators
of $\theta$. We take UNIF as the benchmark in handling big data, because the uniform sampling
involved does not reflect any information about the big data. Its most obvious advantage is requiring nearly no extra calculation cost. An unequal probability sampling does not make sense for big data analysis if the resulting estimator is inferior to the UNIF-based estimator. Figure 1 shows that ELW, ELWAI, and IPW all outperform UNIF in terms of MSE uniformly for all \( r \), indicating that the ELW- and IPW-based two-step unequal probability samplings seem to be meaningful. Moreover, both ELW and ELWAI outperform IPW uniformly for all \( r \), although a shrinkage technique is employed for IPW (Ma et al., 2014) in Examples 1 and 2. This suggests that the proposed ELW estimation and nearly optimal sampling strategy produce better estimators than the IPW estimation and sampling strategy, regardless of whether auxiliary information is used. In particular, the
Figure 2: Plots of the logarithm of MSE versus $r$ for UNIF, IPW, ELW, and ELWAI under the L-criterion.

Estimation efficiency gains of ELW and ELWAI over IPW are remarkable, except in cases 1 and 3 of Example 3. Regarding the two ELW methods, the ELWAI-based estimator gives a uniformly smaller MSE than the ELW-based estimator, especially in case 1 of Example 3. This clearly implies the ELW method can produce more reliable estimators by incorporating auxiliary information, as disclosed by Theorem 2.

When the A-criterion is replaced by the L-criterion, the empirical MSEs in (20) of the generic estimator $\hat{\theta}$ are different from the asymptotic MSEs of the linearly transformed estimator $V\hat{\theta}$. The optimal sampling plan minimizing the latter may not produce a point estimator that has a minimal empirical MSE. Even so, the results in Figure 2 show that the efficiency order of ELW, ELWAI, IPW, and UNIF is the same as in Figure 1 indicating
that the proposed ELW methods uniformly outperform IPW again. Additionally, by incorporating auxiliary information, ELWAI achieves an efficiency gain over ELW. One benefit of using the L-criterion is that ELW, ELWAI, and IPW have much lower computational costs than under the A-criterion.

5.3 Evaluation of our sample size determination methods

In Section 4, we presented two sample size determination methods, M1 and M2, under requirements (R1) and (R2), respectively. With the sample sizes determined by M1 and M2, we now examine whether the proposed sampling and estimation strategy produces estimators that have the desired precision. To this end, we fix the first-capture sample size to \( r_0 = 200 \) and determine the second-capture sample size \( \tilde{r} \) by \( \tilde{r} = N(\tilde{n}_0 - r_0)/(N - r_0) \) for the ELW method, where \( \tilde{n}_0 \) is the root of (18) under requirement (R1) or (19) under requirement (R2), where \( a = 5\% \).

We consider 10 distinct values of \( C_0 \) or \( d_0 \) for each case, so that \( \tilde{r} \) ranges from 300 to 2000. To ensure a fair comparison, we apply ELWAI and IPW with same sample size pair \((r_0, \tilde{r})\), namely the ideal size of the initial sample is \( r_0 \) and that for the second sample is \( \tilde{r} \). When applying UNIF, we set the total sample size to be \( r_0 + \tilde{r} \). For a generic estimator \( \hat{\theta} \), we calculate the ratio of its actual MSE to the specified \( C_0 \), and simulate the coverage probabilities of \( \{ \theta : \| \hat{\theta} - \theta \| \leq d_0 \} \) based on 500 simulated repetitions. The results are displayed in Figure 3 where each box-plot is based on 10 ratios (upper panel) or simulated coverage probabilities (lower panel).

In the upper panel, the ratios based on ELW are all close to or less than 1. In other words, with the sample size determined by M1, the MSE of the ELW-based estimator is close to (and no greater than) the prespecified precision \( C_0 \). The sample size is quite
Figure 3: Ratios of actual MSEs to $C_0$ under requirement (R1) (upper panel) and simulated coverage probabilities under requirement (R2) (lower panel) with $1 - a = 95\%$. ELW (red), ELWAI (green), IPW (blue), and UNIF (purple) correspond to columns 1–4 from left to right in each case.

accurate under Examples 1 and 2 because the ratios are quite close to 1, although it is somewhat conservative in cases 1–3 of Example 3, where the ratios are no greater than 75%. The ratios based on ELWAI are always slightly smaller than those based on ELW, which makes sense as the ELWAI-based estimator is more efficient than the ELW-based estimator, both theoretically and numerically. The ratios based on IPW and UNIF are much greater than 1, which coincides with the observation that they both are less efficient than ELW.

In the lower panel, the coverage probabilities corresponding to ELW are always close to or greater than 95%, as specified by requirement (R2). Thus, with the sample size
determined by M2, the confidence region \( \{ \theta : \| \hat{\theta}_{\text{ELW}} - \theta \| \leq d_0 \} \) has coverage probabilities no less than the prespecified confidence level of 95%. With the same sample size, the ELWAI-based confidence region has an even greater coverage probability, because the ELWAI-based estimator is more efficient than the ELW-based estimator. However, the IPW- and UNIF-based confidence regions have much low coverage probabilities, which are often no greater than 90%. In all cases, the boxplots of ELW and ELWAI are much shorter than those of IPW and UNIF, suggesting that ELW and ELWAI provide much more stable performance than IPW and UNIF.

Overall, M1 and M2 usually produce reasonable sample sizes with which the ELW method approximately meets target requirements (R1) and (R2), respectively. The inferior performance of IPW and UNIF in Figure 3 indicates that many more samples are usually required to achieve the same estimation precision compared with ELW and ELWAI.

6 Applications

In this section, we further investigate the performance of the proposed ELW estimation and nearly optimal capture–recapture sampling method by analyzing three real datasets: a bike sharing dataset, an income dataset, and a protein structure dataset, as found in the supplementary material of Yao and Wang (2021).

The bike sharing dataset consists of 17,379 observations, in which we take the number of bikes rented hourly as the response. The covariates include a binary variable \( X_1 \), indicating whether a certain day is a working day or not, and the three continuous variables of temperature \( (X_2) \), humidity \( (X_3) \), and windspeed \( (X_4) \). The income dataset contains 48,842 observations, in which the response is a binary variable indicating whether one person’s income is over 50,000 $ or not. Five continuous covariates are considered, namely...
the person’s age, weight, education, capital loss, and working hours per week, denoted as \( X_1 - X_5 \), respectively. The protein structure dataset contains 45,730 observations, where the 75-th percentile of the size of the residue ranging from 0 to 21 Angstrom may be affected by eight covariates \((F_1, F_2, F_4 - F_9)\), denoted as \( X_1 - X_8 \).

To investigate the relationship between the responses and the covariates, we fit a Poisson regression model, a logistic regression model, and a quantile regression model with \( \tau = 0.75 \) to the three datasets, respectively. To eliminate the influence of scales of different variables, we centralize and standardize the covariates in all datasets and the response variable in the protein structure dataset. The regression coefficients of the regression models based on the full datasets are reported in Table 2.

| Data               | Model            | Intercept | \( X_1 \) | \( X_2 \) | \( X_3 \) | \( X_4 \) | \( X_5 \) | \( X_6 \) | \( X_7 \) | \( X_8 \) |
|--------------------|------------------|-----------|------------|------------|------------|------------|------------|------------|------------|------------|
| Bike sharing       | Poisson regression | 5.02      | 0.03       | 1.83       | -1.36      | 0.20       |            |            |            |            |
| Income             | Logistic regression | -8.59     | 0.05       | 6E-7       | 0.34       | 6E-4       | 0.04       |            |            |            |
| Protein structure  | Quantile regression | 0.62      | 0.89       | 0.87       | -1.27      | -0.38      | -0.38      | -0.04      | 0.26       | -0.10      |

We apply the UNIF, IPW, ELW, and ELWAI methods to the three real datasets. The remaining settings, such as sample sizes and number of simulation repetitions, are the same as those in Section 5.2. Figure 4 displays the logarithms of the empirical MSEs of a point estimator versus the sample size \( r \) of the second-step sampling. Clearly, ELW, ELWAI, and IPW outperform the naive method, UNIF, by a large margin when the A-criterion is used to construct the optimal sampling design. The proposed ELW- and ELWAI-based estimators both have much smaller empirical MSEs. These findings can also be seen from the results for the bike sharing dataset and the income dataset under the L-criterion, and coincide with those from our simulation studies. What differs is that the efficiency gains of ELWAI over ELW based on the first two datasets are much greater than those in our simulation.
studies. This implies that the auxiliary information of the full-data response contains more information, and is thus more helpful in improving the performance of ELW in the former than in the latter. Based on the protein structure dataset under the L-criterion, although all four methods have almost the same performance, our ELW and ELWAI are slightly more reliable than IPW and UNIF.

Based on the three real datasets, we also investigate the performance of our sample size determination methods, M1 and M2, under the same settings as in Section 5.3. Again we find that they provide desirable sample sizes that guarantee the ELW and ELWAI methods meet the given estimation precision requirements.

Figure 4: Plots of the logarithm of MSE versus $r$ for UNIF, IPW, ELW, and ELWAI under the A-criterion (upper row) and the L-criterion (lower row) based on the three real datasets.

Based on the three real datasets, we also investigate the performance of our sample size determination methods, M1 and M2, under the same settings as in Section 5.3. Again we find that they provide desirable sample sizes that guarantee the ELW and ELWAI methods meet the given estimation precision requirements.
7 Discussion

Based on a capture–recapture sample from a big dataset, we have developed an ELW estimation method for M-estimation problems. The proposed approach not only overcomes the instability of the conventional IPW estimation method, but also improves the estimation efficiency by incorporating auxiliary information. A nearly optimal capture–recapture sampling plan was constructed accordingly. Theoretically, the ELW method is asymptotically more efficient than the IPW method, which means that the proposed sampling and estimation method requires fewer samples to achieve the target estimation precision. For technical convenience, we assumed the convexity of the loss function in the M-estimation problem. Our ELW estimation method also applies to general M-estimation problems and general estimating equation problems (Qin and Lawless, 1994). Further efforts may be needed to establish the asymptotic normality of the resulting point estimator, which is the foundation for constructing optimal sampling plans.

The capture–recapture sampling we have considered consists of a pilot uniform sampling and a refined sampling. Under this sampling framework, we established two sample size determination methods under estimation precision requirements (R1) and (R2), respectively. These methods are new in the literature of optimal subsampling for big data. They may need to be modified when the parameter of interest is a smooth function of $\theta$, such as $C\theta$ for a given matrix $C$, rather than $\theta$ itself. In addition, the current capture–recapture sampling consists of only two subsampling processes, although this may be extended to multiple subsampling processes when needed.

SUPPLEMENTARY MATERIAL

The supplementary material contains the proofs of Theorems 1–3. (SubsampEL_supp.pdf)
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