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Ranked Set Sampling Based on Binary Water Quality Data With Covariates

Paul H. KVAM

A ranked set sample (RSS) is composed of independent order statistics, formed by collecting and ordering independent subsamples, then measuring only one item from each subsample. If the cost of sampling is dominated by data measurement rather than collection or ranking, the RSS technique is known to be superior to ordinary sampling. Experiments based on binary data are not designed to exploit the advantages of ranked set sampling because categorical data typically are as easily measured as ranked, making RSS methods impractical. However, in some environmental and biological studies, the success probability of a bivariate outcome is related to one or more covariates. If the covariate information is not easily quantified, but can be objectively ordered with respect to this success probability, the RSS method can be used to improve the analysis of binary data. This article considers the case in which the covariate information is modeled in terms of a mixing distribution for the success probability, and the expected success probability is of primary interest. The inference technique is demonstrated with water-quality data from the Rappahannock river in Virginia. In a general setting, the RSS estimator is shown to be superior, including cases in which error in judgment ranking is present.

Key Words: Binomial sampling; Concomitant; Judgment error; Mixture distribution.

1. INTRODUCTION

The ranked set sampling procedure, first suggested by McIntyre (1952), has found economical application where experimental units can be ranked with substantially less effort than making an actual measurement. First, independent and identically distributed items from the population are collected and ordered according to the property of interest. From this ordered *subsample*, only one observation is measured and recorded, along with its rank within the subsample. This is repeated so that the resulting sample consists of independent order statistics. If subsamples have constant size, say k, and each of the k order statistics are sampled in equal proportion across all subsamples, the ranked set sample is said to be balanced.

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Initial work on ranked set sampling was directed toward estimating the unknown population mean. Takahasi and Wakimoto (1968) showed that the mean of a balanced ranked set sample (RSS) is the unique linear unbiased estimator of the population mean, and that the variance of the RSS estimator is less than or equal to the sample mean variance based on a simple random sample (SRS) of the same size. The relative precision (RP) of the RSS estimator with respect to the SRS estimator, (defined as the variance of the SRS mean divided by the variance of the RSS mean) differs according to the underlying distribution of the data, and is bounded above by (k + 1)/2 for continuous distributions, with the upper bound achieved only for the uniform distribution. This improvement gained from ranked set sampling makes intuitive sense because the RSS estimator obtains information from ktimes as many independent subsample units, even though both estimators rely on the same number of actual measurements.

Dell and Clutter (1972) first considered situations of imperfect ranking; that is, the ranking within the subsample might be flawed so that the observation said to be the rth smallest value out of k may be some other order statistic. They showed that the RSS estimator based on these "judgment" order statistics remains unbiased, and the precision is nevertheless improved over the simple random sample mean unless ranking is done randomly, in which case the estimators have equal precision. Naturally, the improvement in precision gained by RSS depends strongly on the amount of ranking error in the procedure. See, for example, Ridout and Cobby (1987).

Stokes and Sager (1988) extended ranked set sampling to problems of estimating the distribution function by showing the empirical distribution function (EDF) based on a RSS is unbiased for estimating the underlying distribution function and has smaller variance than the EDF based on an equal-sized random sample. Kvam and Samaniego (1994) used the method of nonparametric maximum likelihood to estimate the distribution function for general ranked set samples in which balance is not necessarily achieved, and asymptotic properties of the MLE were investigated by Huang (1997). The RSS method has also been extended to estimating variance by Stokes (1980), and general linear estimators of scale and location parameters by Kvam and Samaniego (1993).

Experiments based on discrete data, such as binomial outcomes, are not designed to exploit the advantages of RSS. In typical biological and environmental applications, categorical data are as easily measured as ranked, making RSS methods impractical. However, in some settings, the success probability of a bivariate outcome is related to one or more covariates. If the covariates can be easily quantified and measured, logit models might be used to relate the success probability to the covariate data. This supplemental information may not be assessable due to physical constraints or exorbitant expense. If test subjects can be ordered in terms of success probability based on covariate information, we will find that RSS methodology can improve the analysis of the binary data.

In this article, the RSS technique is extended to binomial sampling for the analysis of binary water quality data. Suppose we observe a binomial outcome X based on m independent Bernoulli trials with success parameter p. Although p is not observable in general, we assume it is functionally related to covariates in such a way that test items

can be ranked according to their underlying success probability. For water quality data, the binary outcome is based on whether the total dissolved solids in the river exceeds 50 mg/l, and a measurement of solid residue on evaporation serves as a potential explanatory variable. To model the variability between seasonal time periods, we assign P = P(dissolved solids solids secceeds 50 mg/l) a mixing distribution, say G(p) that is fully or partially unknown. If G is a Beta distribution, for example, the marginal distribution of X is beta-binomial. We assume the covariate has an ordinal scale of measurement, so logistic regression does not offer a plausible solution.

RSS is used in other environmental applications. In the cleanup of hazardous waste sites, the high cost of environmental sampling is driven by the expense of laboratory analysis of the soil samples, which severely limits sampling plans at typical sites. Hand-held instruments used for soil sampling in the field can provide surrogate information about contamination that directly correlates with the more expensive lab analysis. Instruments that are unable to accurately measure low-level contamination, for example, can be used to locate high concentration levels, or "hot spots," as discussed by Kvam, Tiwari, and Zalkikar (2000). Lacayo, Neerchal, and Sinha (2001) presented an example where soil samples are analyzed for plutonium concentration. They noted that levels of Americium in the soil correlate highly with the plutonium concentrations, and Americium levels can be measured using a hand-held device that is substantially less expensive than a standard soil analysis for plutonium. In this example, analysts record the number of independently sampled plots for which plutonium concentration exceeds an upper threshold, so statistical analysis is based on binomial outcomes with surrogate information. Lacayo et al. (2000) suggested a ranked set sampling plan based on the binomial outcomes, which is discussed in the following section.

Other potential applications are generated from agricultural experiments, bioassays, clinical trials, and reliability testing. If an indirect bioassay has a binary response, the test subject might be a living specimen that contains surrogate information related to health (e.g., size, age, appearance) that suggests an order in success (e.g., survival or restoration) probability. For such applications, it may be that the covariate information is available only at great cost to the experimenter, but ranking the test subject according to the covariate information is relatively inexpensive.

In manufacturing, test items generated from different manufacturing processes can give rise to a natural mixing distribution for P, and variability might be revealed in simple signs of quality that are easily ordered, but not easily quantified. The mixing distribution also helps model over dispersion in the data, and has been applied in inferences regarding discrete samples for such purposes. Mixtures are commonly implemented in the analysis of binary data in the life sciences. For instance, teratogenic data can be modeled in this way to allow correlation between responses among littermates, as proposed by Williams (1975).

In the following section, the ranked set sample estimator of a binomial proportion is investigated and compared to the analogous estimator based on a simple random sample. Because ranking involves experimental units with ambiguous covariates, errors in ranking are plausible in many settings, especially if subsamples are allowed to increase to sizes of four or more. Section 3 models judgment error additively, allowing for error to increase in order statistics with larger variances. Conditions are investigated for which judgment error still allows improvement in precision using ranked set sampling. The water quality data are analyzed in Section 4, which helps to demonstrate the RSS method.

2. ESTIMATION OF PROPORTION

From a simple random sample (SRS), let Y_i represent the number of successes (in m trials) of the *i*th observed test item, with i = 1, ..., N. Then the mean success rate $p_0 = E_G(P)$ is estimated using the sample success proportion $(mN)^{-1} \sum_{i=1}^{N} Y_i$, which is unbiased and has variance

$$\frac{p_0(1-p_0)}{Nm} + \frac{(m-1)\sigma_0^2}{Nm},$$
(2.1)

where σ_0^2 denotes the variance of the mixing distribution.

If k such items are collected together, it may be possible to order them according to these success probabilities; that is, if P_1, \ldots, P_k represent k independent realizations from G(p), then $P_{1:k} < \cdots < P_{k:k}$ represent the ordered values for the k different items. If ordering the item according to its success probability is easy relative to generating binomial outcomes from the systems, we will see that ranked set sampling can be used to improve estimation of the mean success rate $p_0 = E_G(P)$ and other properties of the mixing distribution. Although we will assume the set P_1, \ldots, P_k may be ordered, we do not assume any values from G can actually be measured. In realistic applications, this ranking will be subject to some form of judgment error, which is investigated in the following section. Perfect ranking is assumed here for the purpose of simplifying the explanation of the RSS estimators and their properties.

To achieve the ranked set sample, we collect k items, order the success probabilities, and measure the outcome of a single binomial outcome from the ordered set. If the item with rth smallest success probability $P_{r:k}$ is selected, then the number of successes, denoted $X_{[r:k]}$, is not an order statistic, but a concomitant value corresponding to $P_{r:k}$. If we assume we have n copies of each such concomitant outcome, then we can denote the balanced ranked set sample as $\{X_{[r:k]i}, 1 \le r \le k, 1 \le i \le n\}$. The RSS estimator for p_0 is $\hat{p}_0 = (mnk)^{-1} \sum_{i=1}^n \sum_{r=1}^k X_{[r:k]i}$.

To compare the RSS estimator to the SRS estimator, we assume N = nk. If $P_{r:k}$ represents the *r*th smallest observation out of *k* that are generated from an absolutely continuous distribution G(p), we denote the mean and variance of the order statistic as $\bar{p}_{[r:k]}$ and $\sigma^2_{r:k}$, respectively.

Theorem 1. The RSS estimator $\hat{p}_0 = (mnk)^{-1} \sum_{i=1}^n \sum_{r=1}^k X_{[r:k]i}$ is unbiased for p_0 with smaller variance than the SRS estimator, which we shall write $\tilde{p} = (mnk)^{-1} \sum_{i=1}^{nk} Y_i$.

Proof: Takahasi and Wakimoto (1968) showed that if G is continuous, $\sum_{r=1}^{k} \bar{p}_{r:k} = kp_0$, and $\sum_{r=1}^{k} \sigma^2_{r:k} = k\sigma_0^2 - \sum_{r=1}^{k} (\bar{p}_{r:k} - p_0)^2$. From the properties of conditional

variance, the variance of the RSS estimator can be written as

$$\operatorname{var}(\hat{p}_{0}) = (m^{2}nk)^{-1} (E[\operatorname{var}(X_{[r:k]}|P_{r:k})] + \operatorname{var}[E(X_{[r:k]}|P_{r:k})])$$

$$= (m-1)(mnk^{2})^{-1} \sum_{r=1}^{k} \sigma_{r:k}^{2} + (nmk^{2})^{-1} \sum_{r=1}^{k} \bar{p}_{r:k}(1-\bar{p}_{r:k})^{2}$$

$$= (m-1)(mnk)^{-1}\sigma_{0}^{2} + (mnk)^{-1}p_{0}(1-p_{0}) - (nk^{2})^{-1} \sum_{r=1}^{k} (\bar{p}_{r:k}-p_{0})^{2}$$

$$\leq p_{0}(1-p_{0})/(mnk) + (m-1)\sigma_{0}^{2}/(mnk) = \operatorname{var}(\tilde{p}_{0}). \quad (2.2)$$

The amount of savings gained in precision due to ranked set sampling is characterized fully by the relative precision (RP), which can be expressed:

$$RP = \frac{\operatorname{var}(\tilde{p}_{0})}{\operatorname{var}(\hat{p}_{0})}$$

$$= 1 + \frac{m\sum_{r=1}^{k} (\bar{p}_{r:k} - p_{0})^{2}}{kp_{0}(1 - p_{0}) + k(m - 1)\sigma_{0}^{2} - m\sum_{r=1}^{k} (\bar{p}_{r:k} - p_{0})^{2}}$$

$$= 1 + \frac{\sigma_{0}^{2} - k^{-1}\sum_{r=1}^{k} \sigma_{r:k}^{2}}{m^{-1}(p_{0}(1 - p_{0}) - \sigma_{0}^{2}) + k^{-1}\sum_{r=1}^{k} \sigma_{r:k}^{2}}.$$
(2.3)

Theorem 2. With sample size N = nk fixed, the relative precision in (2.3) is an increasing function of m and k.

Proof: It is a matter of routine calculus to show that RP in (2.3) is increasing in m. Also, it is easy to show RP increases as a function of $k^{-1} \sum_{r=1}^{k} \sigma_{r:k}^2$. Theorem 2 in Takahasi and Wakimoto (1968) states that $k^{-1} \sum_{r=1}^{k} \sigma_{r:k}^2$ is a decreasing function of k, thus the theorem holds via the chain rule.

Through calculus of variations, it was shown by Takahasi and Wakimoto (1968) that $(k+1)\sum_{r=1}^{k} (\bar{p}_{r:k} - p_0)^2 \le k(k-1)\sigma_0^2$, with equality obtained if and only if *P* has the Uniform(0,1) distribution, thus the RP in (2.3) is maximized if *P* is distributed U(0,1). For the Uniform distribution, this upper bound of relative precision is

$$RP \le 1 + \frac{m(k-1)}{2(m+k+1)},\tag{2.4}$$

which only achieves the previous (nonmixture) RSS bound of (k + 1)/2 in the limit as m increases to infinity. For Bernoulli outcomes, where m = 1, the effect of variance in the mixing distribution is understood only through the dispersion of expected order statistics in $\sum_{r=1}^{k} (\bar{p}_{r:k} - p_0)^2$.

The RSS procedure produces improved precision for other distributions, which can be much less than the bound in (2.4). For the power-function distribution, with probability density function

$$f(x;\alpha) = \alpha x^{\alpha-1}, \qquad x > 0, \quad \alpha > 0, \tag{2.5}$$

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it can be shown (e.g., Malik 1967) that for values of $1 \le r \le k$, $E(X_{r:k}) = \Gamma(k+1)\Gamma(r+1/\alpha)/(\Gamma(k+1+1/\alpha)\Gamma(r+1))$, thus RP values in (2.3) can be calculated for various values of k and $\alpha > 0$. It can be shown that as the power function becomes more skewed (and thus less disperse), the relative precision decreases considerably.

If P is distributed more generally as $Beta(\alpha, \beta)$, the relative precision decreases at values of (α, β) away from (1,1) at different rates. From (2.2), we can show that if mk is fixed, the RSS estimator variance is minimized by choosing m = 1, meaning that if there is no additional cost associated with sampling test items, it is preferable to test two units just once rather than testing the same unit twice.

A similar RSS technique for dichotomous data was suggested for environmental sampling by Lacayo et al. (2001), where the order of the covariates determines the order of the binary outcomes. This deterministic ordering makes the inference analogous to a missing data problem. Americium concentrations in the soil, corresponding directly to plutonium levels, can be measured without great expense. Plutonium levels are measured through an indicator variable for samples that exceed an upper threshold value. The ordered samples imply a corresponding ordered set of binary outcomes, thus if a field measurement from a sample of k with the highest Americium content does not exceed the plutonium concentration threshold (i.e., $X_{k:k} = 0$), then none of the other k - 1 samples will either. The subsequent inference problem is quite different than the one described in this article.

3. JUDGMENT ERROR

Because the binomial probabilities are not directly measurable, ranking test items according to this criteria generally leads to ranking errors, or "judgment errors." Since Dell and Clutter's (1972) article on imperfect ranking, this problem has received significant attention in the RSS literature. To model judgment error, we assume each ordered probability, $P_{r:k}$, is subject to error in proportion with its natural variability. Let $Q_{r:k} = P_{r:k} + \epsilon_{r:k}$ represent the perceived probability, where $\epsilon_{r:k}$ is an independent random variable in [0,1) with $E(\epsilon_{r:k}) = 0$ and $var(\epsilon_{r:k}) = \omega \sigma^2_{r:k}$ for some constant $\omega \ge 0$. Then $E(Q_{r:k}) = \bar{p}_{r:k}$, and $var(Q_{r:k}) = (\omega + 1)\sigma^2_{r:k}$. In applications of interest, it may be reasonable to assume $\omega < 1$. In this sampling scenario, m > 1 is required for the mean and variance of the mixing distribution to be uniquely identified, because Bernoulli outcomes allow for the identification of only one parameter.

Theorem 3. Let V_{JE} be the RSS estimator variance under judgment error with $\omega > 0$. The RSS estimator is unbiased with $var(\hat{p}_0) \leq V_{\text{JE}} \leq var(\tilde{p}_0)$, the right-hand inequality holding if m > 1 and

$$\omega \le \frac{m \sum_{r=1}^{k} (\bar{p}_{r:k} - p_0)^2}{(m-1) \sum_{r=1}^{k} \sigma_{r:k}^2} \le \frac{m \sum_{r=1}^{k} (\bar{p}_{r:k} - p_0)^2}{(m-1)(k\sigma_0^2 - \sum_{r=1}^{k} (\bar{p}_{r:k} - p_0)^2)}.$$
(3.1)

Proof: We write $V_{\text{IE}} = (mk^2n)^{-1} \sum_{r=1}^{k} (E[Q_{r:k}(1-Q_{r:k})] + mvar[Q_{r:k}])$ which can be simplified to $(mnk)^{-1}(m-1)(\omega+1)\sigma^2_0 + (mnk)^{-1}p_0(1-p_0) - (nk^2)^{-1}(1+\omega)^{-$

ROE	Rank	$I(TDS \ge 50)$	ROE	Rank	$I(TDS \ge 50)$
63	1st	1	54	3rd	0
56	2nd	0	45	4th	0
54	3rd	0	55	1st	0
50	4th	0	56	2nd	1
62	1st	0	45	3rd	0
48	2nd	0	43	4th	0
49	3rd	0	69	1st	1
48	4th	0	50	2nd	1
52	1st	0	56	3rd	0
59	2nd	1	38	4th	0

Table 1. Ranked Set Sample Measurements for Residue on Evaporation (ROE) and Total Dissolved Solids (TDS) Data from Rappahannock River, Virginia, 1978ñ1989

 $m^{-1}(m-1)\omega \sum_{r=1}^{k} (\bar{p}_{r:k} - p_0)^2$. Clearly, the RSS estimator remains unbiased, and the left-hand inequality is satisfied for $\omega \in [0, 1]$. Finally, $V_{\text{JE}} \leq \text{var}(\tilde{p}_0)$ if and only if $k^{-2}(1 + m^{-1}(m-1)\omega) \sum_{r=1}^{k} (\bar{p}_{r:k} - p_0)^2 \geq (mk)^{-1}(m-1)\omega\sigma_0^2$, which is equivalent to (3.1).

If P is distributed U(0, 1), Theorem 1 states that relative precision is increased with ranked set sampling provided the error ω bounded above by 0.5m(k-1)/(m-1). In most cases, it would be reasonable to assume $\omega < 1$, so this bound is assured if k > 2. For the power-function distribution, the bound in (3.1) can also be iterated in terms of relative precision:

$$\omega \le \frac{m}{m-1} (\mathbf{R}\mathbf{P}^{\infty} - 1), \tag{3.2}$$

where RP^{∞} is the relative precision (thus $RP^{\infty} - 1$ is the relative improvement in precision) for the power function distribution if $m = \infty$.

4. EXAMPLE

Stream water quality data from the National Stream Quality Accounting Network (NASQAN) station on the Rappahannock River near Fredricksburg, VA, are listed in Table 1. This table, summarized from Helsel and Hirsch (1991), is comprised of measurements of solid residue on evaporation (ROE), measured in mg/l, and an indicator for the event that the total dissolved solids (TDS) level exceeds 50 mg/l. The data are grouped into homogeneous (seasonal) time periods. The first ROE measurement is the largest from a subsample of four, the second is the second largest from another subsample of four, and so on. The presence of TDS in the water is of primary interest in the study.

If the ROE is measured on an interval scale in such a way that the correlation between ROE and TDS can be established, a logistic regression would be more appropriate than the binary data analysis that follows. However, in this case we assume the ROE measurements are only valid for distinguishing the order of TDS in the water quality measurements, and the measure of 63 mg/l in the first sample tells us only that the other three ROE measurements during that seasonal time period were less than 63.

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We know the estimate of the proportion of sample measurements for which TDS exceeds the upper threshold ($\hat{p}_0 = 5/20 = 0.25$) is inherently more precise than a simple random sample estimator based on the same number of measurements. However, the uncertainty of \hat{p}_0 is concealed by the unknown G(p). If we allow G(p) to be a Beta distribution with mean \hat{p}_0 and largest allowable dispersion in (0, 1), a conservative estimate of $var(\hat{p}_0)$ can be computed and used for uncertainty bounds for p_0 . Following Berger's (1985) suggestion for maximizing disperseness of prior distributions, we choose the Beta density g(p) that maximizes the Shannon–Jaynes entropy among all such densities for which $p_0 = \hat{p}_0$:

$$H(g) = -\int_0^1 g(p)ln(g(p))dp.$$

Numerically, we can maximize the functional H(g) based on $g(p) \sim \text{Beta}(\alpha, \beta)$, with $\alpha = 0.392$ and $\beta = 1.176$. From (2.2), our estimate of $\text{var}(\hat{p}_0)$ is 0.007553 ($\hat{\sigma}_{\hat{p}_0} = 0.0869$). A similar maximum-entropy program was constructed for a binary-data reliability study by Savchuck and Martz (1994). For the water-quality example, the estimated relative precision from (2.3) is 1.24, so a confidence interval based on a simple random sample (which ignores the covariate information provided by the ranked ROE) is 11.4% larger than a confidence interval based on the RSS.

5. DISCUSSION

Section 2 establishes that ranked set sampling can be used in environmental sampling problems to improve the analysis of binary data. In cases where errors in ranking can occur, the improvement is still certain unless the ranking is done by randomly choosing from the subsample. Other applications, including those from life testing and reliability can exploit the potential improvement in ranked set sampling so long as the test items contain valid surrogate information that allows items to be ordered in terms of success likelihood.

Extensions to general problems of parameter estimation and mixing distributions depend on the relationship between the conditional distribution of the observed data and the mixing distribution. Specifically, the potential improvement gained by sampling independent order statistics depends on the relationship between the variance of the observed outcomes and the mixing distribution. In the case of binomial sampling, the link between the variance and G(p) is a simple function of p, and the resulting mixture distribution is manageable.

Unbalanced ranked set samples can also be considered. In biased experiments, for example, the test item selected from the subsample of size k might always appear to be the largest one, meaning $X_{[k:k]}$ is always drawn for inference regarding p_0 . This is a common sampling practice in environmental studies where contamination is rare and appears in few samples. Naturally, the RSS estimator listed in Theorem 1 is biased using this sampling scheme. Willemain (1980) called this nomination sampling. If the mixing distribution is the power-function distribution listed in (2.5), then $P_{k:k}$, the success probability of the selected test item, is distributed as Beta($k\alpha$,1), and the marginal distribution of an experimental

outcome (based on *m* independent trials) is Beta-binomial($m, k\alpha, 1$). Estimating α or p_0 can be achieved iteratively via method of maximum likelihood, as in Griffiths (1973).

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