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PREFACE

This special issue features specially invited papers from those who presented at the International Conference on Advances in Interdisciplinary Statistics and Combinatorics (AISC 2018) held at the University of North Carolina – Greensboro, USA, during October 5–7, 2018.

The contributions to this special issue cover several very significant areas of statistics such as Randomized Response Models, Small Area Estimation, Genetics, Statistical Tests, Distribution Theory, and Spatial Statistics.

The guest editors are grateful to the contributors to this issue as well as the editors of REVSTAT for their support during the review process. We also wish to acknowledge the help of the referees who reviewed the papers very promptly and diligently.

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SIMULTANEOUS INFERENCE OF GENE ISOFORM EXPRESSION FOR RNA SEQUENCING DATA

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Abstract:

- In this article, we describe simultaneous inferential methods in detecting differentially expressed gene isoforms based on the Poisson generalized linear models. We derive the joint asymptotic distribution of pivotal quantities. The sample size of RNA sequencing data is often small in practice. Using multiple comparison procedures based on large-sample approximation becomes problematic. The parametric bootstrap method based on pivotal quantities is outlined as a robust alternative. Moreover, we observe the validity of robustness of the bootstrap method when mild overdispersion presents in RNA-sequencing data. We demonstrate the validity of the proposed method in detecting differentially expressed isoforms through Monte Carlo simulation. It shows the proposed method controls the family-wise error rate for large-scale inference. Even though the proposed method can be extended to many experimental designs, we focus on factorial designs in this article.

Key-Words:

- *RNA sequencing data; simultaneous inference; parametric bootstrap.*

1. INTRODUCTION

Studies of Gene isoform expression have not only been concentrated on detecting differentially expressed genes with known gene bank ID but also their isoforms due to the development of RNA sequencing technology. RNA sequencing technology, also known as Next Generation Sequencing (NGS), counts how many copies of nucleotide sequence for hundreds to thousands of gene isoforms.

To detect which genes are differentially expressed among hundreds even thousands of genes, researchers often conduct large-scale multiple hypotheses tests simultaneously, see Dudoit *et al.* [3]. One of the major concerns of gene expression analysis is to control the family-wise error rate (FWER). When the multiplicity is overlooked, researchers may claim dozens even hundreds of genes which are differentially expressed but in fact, they are false positives. Concerted efforts have been devoted to controlling FWER for microarray gene expression analysis. Dudoit *et al.* [4] applied Westfall and Young step-down method (Westfall and Young, [13]) based on two-sample Welch's t-tests to detect differentially expressed genes in microarray experiments. Alternatively, simultaneous confidence intervals based on the linear models of Kerr *et al.* [7] are constructed, see Hsu *et al.* [6]. Li and Mansouri [8] proposed simultaneous rank tests to search differentially expressed genes when microarray data violate normality assumption and contain a large number of outliers.

Auer and Doerge [1] proposed factorial designs for RNA sequencing experiments. To account for a variety of sources of variations, the resulting observations are fit to the Poisson generalized linear models, see Auer and Doerge [1]. Under this framework, we propose the simultaneous testing procedure to detect differentially expressed gene isoforms such that it controls FWER. Simultaneous test based on large-sample approximation is outlined. The sample size for RNA sequencing study is often small. As it will be shown in Section 4 that the large-sample approximation method does not provide a satisfactory solution in terms of controlling FWER. Monte Carlo simulation of Mansouri and Li [9] shows that percentile-t bootstrap method based on pivotal quantities provides a viable method in microarray gene expression analysis. Extension of bootstrap method to RNA sequencing gene expression analysis is hence appealing. In this article, we propose the simultaneous inferential method based on pivotal quantities to detect differentially expressed isoforms using parametric bootstrap. We investigate the performance of the proposed method in controlling the overall error rates through a simulation study.

2. PROBLEM FORMULATION AND PIVOTAL QUANTITIES

2.1. Experimental design and generalized linear model

To account for different sources of variations in observations from treatment, batch, flow cell, and lane, we consider factorial designs for the Next Generation Sequencing. In brief, bar-coded mRNA samples are pooled and assigned to different lanes of a sequencing device in such a way that there are n biological replicates randomly assigned at each combination of treatment, lane, and flow cell. For details, see Auer and Doerge [1]. Since we can assign an ID to each isoform sequence in RNA sequencing data file, we may use the term "gene" instead of "isoform" in the following.

For gene l, $l = 1, ..., g$ we let Y_{lijkm} be the the count of readings from the i-th treatment, the j-th flow-cell, the k-th lane, and the m-th biological replicate, $i = 1, ..., a$, $j = 1, ..., b$, $k = 1, ..., c$, and $m = 1, ..., n$. We assume Y_{lijkm}'s are independent random observations and the expected value $E(Y_{lijkm}) = \mu_{lijk}$, for $m = 1, ..., n$ follow a per gene Poisson model with log-link (Auer and Doerge, [1]) that

$$\log(\mu_{lijk}) - \log(c_{jk}) \;=\; \alpha_l + \tau_{li} + \nu_{lj} + \omega_{lk} \tag{2.1}$$

where α_l is the overall gene l effect; τ_{li} is the i-th treatment effect on gene l with $\sum_i \tau_{li} = 0$; ν_{lj} is the j-th flow cell effect on gene l with $\sum_j \nu_{lj} = 0$; ω_{lk} is the k-th lane effect on gene l with $\sum_k \omega_{lk} = 0$; c_{jk} is a known constant, namely library size, $j = 1, ..., b$, $k = 1, ..., c$ to normalize the readings from j-th flow-cell and k-th lane, see Section 6 and Chen *et al.* [2]. We assume that $\alpha_l, \tau_{li}, \nu_{lj}, \omega_{lk}$, for $l = 1, ..., g$, $i = 1, ..., a$, $j = 1, ..., b$, and $k = 1, ..., c$ in (2.1) are fixed effects. Let $N = abcn$ be the total number of readings from each gene.

We let vector

$$\mathbf{Y}_l \;=\; \Big[Y_{l1111}, ..., Y_{l111n}, ..., Y_{lijk1}, ..., Y_{lijkn}, ..., Y_{labc1}, ..., Y_{labcn}\Big]'$$

be a collection of all readings from gene l and let $\boldsymbol{\mu}_l = E(\mathbf{Y}_l)$, $l = 1, ..., g$. It is useful to write the model in (2.1) in the form of matrix representation that

$$\log(\boldsymbol{\mu}_l / c_{jk}) \;=\; X\boldsymbol{\beta}_l \tag{2.2}$$

where $\boldsymbol{\beta}_l = \big[\alpha_l, \tau_{l1}, ..., \tau_{l(a-1)}, \nu_{l1}, ..., \nu_{l(b-1)}, \omega_{l1}, ..., \omega_{l(c-1)}\big]'$ and X is the corresponding $N \times (a + b + c - 2)$ design matrix.

Since we use per gene generalized linear model, the model for all genes can be written as

$$\mathbf{1}_g \otimes \log(\boldsymbol{\mu}_l / c_{jk}) \;=\; \mathbf{1}_g \otimes X\boldsymbol{\beta}_l\,. \tag{2.3}$$

2.2. Pivotal quantities

For gene l, $l = 1, ..., g$ we assume

$$Y_{lijkm} \sim \text{Poisson}(\mu_{lijk})\,, \qquad \text{for} \quad m = 1, ..., n\,, \tag{2.4}$$

where

$$\mu_{lijk} \;=\; \exp\big[(\alpha_l + \tau_{li} + \nu_{lj} + \omega_{lk}) + \log(c_{jk})\big] \tag{2.5}$$

with $i = 1, ..., a$, $j = 1, ..., b$, $k = 1, ..., c$, and $m = 1, ..., n$.

Let $\widehat{\boldsymbol{\beta}}_{l,N}$ be the maximum likelihood estimation of $\boldsymbol{\beta}_l$, $l = 1, ..., g$. We apply Newton–Raphson method using Fisher Scoring to compute the estimation. We may suppress the notation of the dependence on N and denote the estimation by $\widehat{\boldsymbol{\beta}}_l$.

Now, we define a $q \times (a+b+c-2)$ comparison matrix C to detect differential gene expression among treatments. In gene expression studies, researchers often interest in i) all-pairwise comparisons of gene expression over treatments, or ii) comparing gene expression for several treatments versus a control, Hsu *et al.* [6]. We focus on all-pairwise comparisons in this article and analogous results should hold for multiple comparisons to a control. As an example of comparison matrix C for all-pairwise comparisons, see (4.1) in Section 4.

Let W_l be $N \times N$ diagonal weight matrix whose diagonal elements are given by μ_{l1111}, ..., μ_{l111n}, ..., μ_{lijk1}, ..., μ_{lijkn}, ..., μ_{labc1}, ..., μ_{labcn} in order. The vector containing pivotal quantities is given by

$$\boldsymbol{T}(\boldsymbol{\beta}_l) = \Sigma_l^{-1/2}\big[C(\widehat{\boldsymbol{\beta}}_l - \boldsymbol{\beta}_l)\big] \tag{2.6}$$

where Σ_l is a diagonal matrix whose diagonal elements equal to the diagonal elements in $C(X'W_lX)^{-1}C',\ l = 1, ..., g$.

In relation to the Poisson generalized linear model in (2.3), (2.4), and (2.5), consider gene expression by letting

$$\boldsymbol{T}(\boldsymbol{\beta}) = \big[\boldsymbol{T}(\boldsymbol{\beta}_1)', ..., \boldsymbol{T}(\boldsymbol{\beta}_l)', ..., \boldsymbol{T}(\boldsymbol{\beta}_g)'\big]'.$$

The joint limiting distribution of $\boldsymbol{T}(\boldsymbol{\beta})$ is given by the following Theorem.

Theorem 2.1. *Suppose* $\mathbf{Y}_1, ..., \mathbf{Y}_g$ *are independent vectors, for* $\frac{1}{N}(X'W_lX) \overset{N\to\infty}{\longrightarrow} \mathcal{W}_l$, *which is positive definite, for* $l = 1, ..., g$, *then*

$$\sqrt{N}\,\boldsymbol{T}(\boldsymbol{\beta}) \xrightarrow{D} \mathrm{MVN}(\mathbf{1}_g \otimes \mathbf{0}_q, \Lambda), \qquad \text{as} \quad N \to \infty, \tag{2.7}$$

where Λ *is a* $gq \times gq$ *block diagonal matrix such that the* l*-th* $(q\times q)$ *diagonal block matrix* $\Lambda_l = \lim_{N\to\infty} N\Sigma_l^{-1/2}C(X'W_lX)^{-1}C'\Sigma_l^{-1/2},\ l = 1, ..., g$.

Proof of Theorem 2.1 immediately follows equation (5.25) and (S.17) of McCulloch *et al.* [10]. Note: since Λ_l is unknown in practice, we use a consistent estimator $\widehat{\Lambda}_l = N\widehat{\Sigma}_l^{-1/2}C(X'\widehat{W}_lX)^{-1}C'\widehat{\Sigma}_l^{-1/2}$ where $\widehat{\Sigma}_l$ is a diagonal matrix whose elements equal to the diagonal elements in $C(X'\widehat{W}_lX)^{-1}C'$, and $\widehat{W}_l$ has diagonal elements given by $\exp\{(\widehat{\alpha}_l + \widehat{\tau}_{l1} + \widehat{\nu}_{l1} + \widehat{\omega}_{l1}) + \log(c_{11})\}$, ..., $\exp\{(\widehat{\alpha}_l + \widehat{\tau}_{li} + \widehat{\nu}_{lj} + \widehat{\omega}_{lk}) + \log(c_{jk})\}$, ..., $\exp\{(\widehat{\alpha}_l + \widehat{\tau}_{la} + \widehat{\nu}_{lb} + \widehat{\omega}_{lc}) + \log(c_{bc})\}$ in order, $l = 1, ..., g$. In the expression, $\widehat{\alpha}_l$, $\widehat{\tau}_{li}$, $\widehat{\nu}_{lj}$, and $\widehat{\omega}_{lk}$ are maximum likelihood estimation of the parameters, $i = 1, ..., a$; $j = 1, ..., b$; $k = 1, ..., c$. Application of the large-sample approximation method is not trivial since the multivariate normal distribution in Theorem 2.1 has mean and variance with dimension $(gq) \times 1$ and $(gq) \times (gq)$ respectively and the total number of genes g, in RNA-sequencing experiments, is typically very large. We propose an Algorithm in Section 4 to reduce the computational burden in RNA-sequencing gene expression analysis.

A challenge besetting RNA-sequencing gene expression analysis may be the overdispersion among counting data, Auer and Doerge [1] and Wang *et al.* [11]. To proceed, we let ϕ_l be the dispersion parameter and overdispersion occurs when $\phi_l > 1,\ l = 1, ..., g$.

It is suggested in Auer and Doerge [1] that statistics for detecting differential gene expression should be scaled by the dispersion parameter. Hence, a sequence of pivotal quantities, considering overdispersion, are given by

$$\boldsymbol{T}(\boldsymbol{\beta}_l, \phi_l) = (\phi_l\Sigma_l)^{-1/2}\big[C(\widehat{\boldsymbol{\beta}}_l - \boldsymbol{\beta}_l)\big]. \tag{2.8}$$

The pivotal quantities in (2.6) can be considered as a special case of (2.8) when $\phi_l = 1$. We focus on gene expression analysis for RNA-sequencing data, which presents mild overdispersion such that ϕ_l is in a neighborhood of 1, and examine the validity of robustness of the large-sample approximation method through a simulation study in Section 4 in this article.

3. SIMULTANEOUS INFERENCE USING BOOTSTRAP

3.1. Simultaneous inference

In relation to the generalized linear model in (2.3), let the relative gene expression be $\tau_{li} - \tau_{li'}$, $i \neq i' = 1, ..., a$, $l = 1, ..., g$. Detecting all-pairwise differential gene expression can be formulated as testing a sequence of hypotheses that:

$$H_{0_{l,ii'}}\colon\ \tau_{li} - \tau_{li'} = 0 \qquad \text{vs.} \qquad H_{1_{l,ii'}}\colon\ \tau_{li} - \tau_{li'} \neq 0 \tag{3.1}$$

for $i \neq i' = 1, ..., a$, $l = 1, ..., g$. Hence we conduct $q \times g$ tests simultaneously, where q is the number of rows in comparison matrix C such that $C\boldsymbol{\beta}_l = [\tau_{l1} - \tau_{l2}, ..., \tau_{l(a-1)} - \tau_{la}]'$, see (4.1) for example.

The resulting test statistics are given by

$$\boldsymbol{T}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l) = (\widehat{\phi}_l \widehat{\Sigma}_l)^{-1/2} C \widehat{\boldsymbol{\beta}}_l \tag{3.2}$$

for $l = 1, ..., g$ where the plug-in estimation of ϕ_l in Auer and Doerge [1] is given by

$$\widehat{\phi}_l = \left(\sum_{i,j,k,m} \frac{\Big(Y_{lijkm} - \exp\big\{(\widehat{\alpha}_l + \widehat{\tau}_{li} + \widehat{\nu}_{lj} + \widehat{\omega}_{lk}) + \log(c_{jk})\big\}\Big)^2}{\exp\big\{(\widehat{\alpha}_l + \widehat{\tau}_{li} + \widehat{\nu}_{lj} + \widehat{\omega}_{lk}) + \log(c_{jk})\big\}} \right) \Big/ \big(N - (a + b + c - 2)\big). \tag{3.3}$$

For gene l, write

$$\boldsymbol{T}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l) = \Big[T_{12}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l), ..., T_{ii'}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l), ..., T_{(a-1)a}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l)\Big]'$$

in association to the hypotheses in (3.1) and the test statistics in (3.2). For all-pairwise comparisons, the total number of comparisons (the total number of elements in $\boldsymbol{T}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l)$) $q = \binom{a}{2}$.

Simultaneous level-α tests reject hypothesis $H_{0_{l,ii'}}$, $i \neq i' = 1, ..., a$, $l = 1, ..., g$ if:

$$\big|T_{ii'}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l)\big| > q_\alpha \tag{3.4}$$

where q_α is the upper α-th quantile of the distribution of maximum modulus statistics $\max\limits_{\substack{i \neq i' = 1, ..., a \\ l = 1, ..., g}} \big\{|T_{ii'}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l)|\big\}$.

When the magnitude of differential gene expression is of interest, a $(1-\alpha)\ 100\%$ simultaneous confidence interval of $\tau_{li} - \tau_{li'}$, $i \neq i' = 1, ..., a$, $l = 1, ..., g$ is given by

$$\boldsymbol{c}'_{ii'} \widehat{\boldsymbol{\beta}}_l \ \pm\ q_\alpha \big\{\widehat{\phi}_l\, \boldsymbol{c}'_{ii'} (X' \widehat{W}_l X)^{-1} \boldsymbol{c}_{ii'}\big\}^{1/2} \tag{3.5}$$

where $\boldsymbol{c}_{ii'}$ is the row vector of C in association to $\tau_{li} - \tau_{li'}$, $i \neq i' = 1, ..., a$ for all $l = 1, ..., g$.

3.2. Bootstrap based on pivotal quantities

It can be shown that the upper α-th quantile of the multivariate normal distribution defined in (2.7) is a consistent estimator of q_α. RNA sequencing data analysis is often complicated by a large number of unknown parameters but a limited number of observations. Using the large-sample approximation method indicated by Theorem 2.1 can be problematic in the estimation of q_α as it will be shown in Section 4. We propose the parametric bootstrap method based on pivotal quantities to approximate quantiles q_α in detecting differentially expressed genes for RNA sequencing data.

For $r = 1, ..., B$, we define the $q \times 1$ vector of pivotal quantities based on the r-th bootstrap sample by

$$\boldsymbol{T}^{(r)}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l) = \left(\widehat{\phi}_l^{(r)} \widehat{\Sigma}_l^{(r)}\right)^{-1/2} C\left[\widehat{\boldsymbol{\beta}}_l^{(r)} - \widehat{\boldsymbol{\beta}}_l\right], \qquad l = 1, ..., g\,, \tag{3.6}$$

where $\widehat{\phi}_l^{(r)}$, $\widehat{\Sigma}_l^{(r)}$, and $\widehat{\boldsymbol{\beta}}_l^{(r)}$ are estimated based on the r-th bootstrap data set. Analogously, we write

$$\boldsymbol{T}^{(r)}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l) = \left[T_{12}^{(r)}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l), ..., T_{ii'}^{(r)}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l), ..., T_{(a-1)a}^{(r)}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l)\right]'.$$

We use the following Algorithm to approximate quantiles q_α. For each r, $r = 1, ..., B$,

(i) for each l, $l = 1, ..., g$ generate random variables $\{Y_{lijkm}\}$ from $\text{Poisson}\big(\exp\{(\widehat{\alpha}_l + \widehat{\tau}_{li} + \widehat{\nu}_{lj} + \widehat{\omega}_{lk}) + \log(c_{jk})\}\big)$, $i = 1, ..., a$, $j = 1, ..., b$, $k = 1, ..., c$, and $m = 1, ..., n$;

(ii) obtain maximum modulus statistics

$$T_M^{(r)}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l) = \max_{i \neq i' = 1,...,a} \left\{\left|T_{ii'}^{(r)}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l)\right|\right\}, \qquad l = 1, ..., g\,,$$

and

$$T_M^{(r)}(\widehat{\boldsymbol{\beta}}, \widehat{\phi}) = \max_{l=1,...,g} \left\{T_M^{(r)}(\widehat{\boldsymbol{\beta}}_l, \widehat{\phi}_l)\right\}.$$

Repeat (i) and (ii) B times, and the upper α-th quantile of the sampling distribution of $T_M^{(r)}(\widehat{\boldsymbol{\beta}}, \widehat{\phi})$ is an approximation of q_α.

As it will be shown in Section 4, the bootstrap method provides a viable alternative of the large-sample approximation method when the overdispersion parameter is in a neighborhood of $\phi_l = 1$, $l = 1, ..., g$.

4. SIMULATION STUDY

In this section, we investigate the performance of the proposed method in terms of controlling the family-wise error rate (FWER) using Monte Carlo simulation.

We assign the following values to the parameters of the model in (2.1). Let

$$\tau_{li} = 0, \quad \text{for } l = 1, ..., 20, \quad i = 1, 2, 3, 4 \quad (\textit{Complete Null})\,,$$

$$\tau_{li} = 0, \quad \text{for } l = 1, ..., 15, \quad i = 1, 2, 3, 4 \quad (\textit{Partial Null})\,.$$

To study the power rates under partial null hypotheses, we let $\tau_{l1} = -0.02$, $\tau_{l2} = 0.01$, $\tau_{l3} = 0.01$, and $\tau_{l4} = 0$, for $l = 16, ..., 20$.

For nuisance parameters, we let $\alpha_l = -3$ and

$$\nu_{lj} = \begin{cases} \ \ 0.5\,, & \text{if} \ \ j = 1\,, \\ -1\,, & \text{if} \ \ j = 2\,, \\ \ \ 0.5\,, & \text{if} \ \ j = 3\,, \end{cases}$$

for $l = 1, ..., 20$. Let

$$\omega_{lk} = \begin{cases} \ \ 0.25\,, & \text{if} \ \ k = 1\,, \\ -0.5\,, & \text{if} \ \ k = 2\,, \\ \ \ 0.75\,, & \text{if} \ \ k = 3\,, \\ -1.25\,, & \text{if} \ \ k = 4\,, \\ \ \ 1.5\,, & \text{if} \ \ k = 5\,, \\ -0.75\,, & \text{if} \ \ k = 6\,, \end{cases}$$

for $l = 1, ..., 20$.

Assume the library size for each lane and flow cell $c_{jk} = 1{,}000{,}000$ for all $j = 1, 2, 3$ and $k = 1, ..., 6$.

We may rewrite the model in (2.1) as $\log(\lambda_{lijk}) = \alpha_l + \tau_{li} + \nu_{lj} + \omega_{lk}$, where the sampling rate $\lambda_{lijk} = E(Y_{lijk}/c_{jk})$ and c_{jk} is a given constant. The observations Y'_{lijkm} are generated from Poisson(μ_{lijk}) where $\mu_{lijk} = c_{jk}\lambda_{lijk}$, for $m = 1, 2$. To exam the performance of the proposed method under mild overdispersion, we add Gaussian noise $\epsilon_{lijkm} \sim N(0, (\phi_l - 1)\mu_{lijk})$ $(\phi_l > 1)$ to the observations that $Y_{lijkm} = Y'_{lijkm} + [\epsilon_{lijkm}]$, $i = 1, ..., 4$, $j = 1, 2, 3$, $k = 1, ..., 6$, $m = 1, 2$ for gene l, $l = 1, ..., 20$ as it is treated in Auer and Doerge [1]. Note that $E(Y'_{lijkm} + \epsilon_{lijkm}) = \mu_{lijk}$ and $\text{Var}(Y'_{lijkm} + \epsilon_{lijkm}) = \phi_l \mu_{lijk}$. We choose $\phi_l = 1.1$, 1.05, 1.01, and 1.001 respectively and let $Y_{lijkm} = Y'_{lijkm}$ for $\phi_l = 1$. In addition, we let the observations equal to zero if it generates "negative" counts, though the chance of generating "negative" counts is rare when the value of $(\phi_l - 1)$ is small.

Hence, the vector of parameters $\boldsymbol{\beta}_l = [\alpha_l, \tau_{l1}, \tau_{l2}, \tau_{l3}, \nu_{l1}, \nu_{l2}, \omega_{l1}, ..., \omega_{l5}]'$, $l = 1, ..., g$. Let X be the corresponding design matrix for all genes. Consider all-pairwise comparisons among treatments. Let C be the 6×11 comparison matrix given by

$$C = \begin{bmatrix} 0 & 1 & -1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & -1 & 0 & \cdots & 0 \\ 0 & 2 & 1 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & 2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 1 & 2 & 0 & \cdots & 0 \end{bmatrix}. \tag{4.1}$$

We run simultaneous tests in (3.4) $1{,}000$ times and compute the empirical overall error rates. Widely used measures of the overall error rates in gene expression analysis are the family-wise error rate (FWER) and the false discovery rate (FDR). Let FWER$_0$ be the probability that at least one true null hypotheses rejected under complete null hypotheses. Let FWER$_1$ be the probability that at least one true null hypotheses rejected under partial null hypotheses. The false discovery rate (FDR) is computed as the average proportion of wrongly rejected null hypotheses among all rejected hypotheses. FDR is defined as 0 if no rejection were made. To investigate the power of the simultaneous tests, we compute the proportional power rate by obtaining the average proportion of genes found differentially expressed among all misexpressed genes, Dudoit *et al.* [3].

To evaluate the performance of the large-sample approximation method, we use the following Algorithm to generate quantiles based on the multivariate normal distribution defined in Theorem 2.1. In specific, for each r, $r = 1, ..., B$,

(i*) generate random variables $\boldsymbol{T}_l^{(r)}$ from $\mathrm{MVN}(\mathbf{0}, \widehat{\Lambda}_l)$, for all $l = 1, ..., g$;

(ii*) obtain maximum modulus statistics $T_{M_l}^{(r)} = \max\{|\boldsymbol{T}_l^{(r)}|\}$, $l = 1, ..., g$ and $T_M^{(r)} = \max\{T_{M_l}^{(r)}\}$.

Repeat (i*) and (ii*) B times, and the upper α-th quantile of the empirical distribution of $T_M^{(r)}$ is an approximation of q_α based on Theorem 2.1.

The performance of the large-sample approximation method and the bootstrap method in the simulation study are summarized in Table 1.

Table 1: Error rates of detecting differentially expressed genes/isoforms — nominal type-1 error rate $\alpha = 0.05$.

Method	ϕ_l	FWER$_0$	FWER$_1$	FDR	Prop. Power
No Adjustment	1.000	0.993	0.970	0.146	—
MVN	1.000†	0.072	0.059	0.003	0.889
	1.050 (1.1)‡	0.084	0.061	0.003	0.861
	1.010	0.073	0.045	0.002	0.887
	1.001	0.065	0.065	0.003	0.886
Bootstrap Method	1.000	0.052	0.037	0.002	0.878
	1.050 (1.1)	0.051	0.035	0.002	0.849
	1.010	0.049	0.034	0.002	0.874
	1.001	0.050	0.045	0.002	0.872

Notes:

i) Simulation size = 1,000. Bootstrap size $B = 200$.
ii) FWER$_0$ denotes the family-wise error rate under complete null hypotheses.
iii) FWER$_1$ denotes the family-wise error rate under partial null hypotheses.
iv) MVN denotes the method of large-sample approximation in Section 3.1.
v) "Bootstrap Method" means the parametric bootstrap method in Section 3.2.
vi) † The same value of ϕ_l is assigned to all genes.
vii) ‡ The first 15 genes have $\phi_l = 1.05$ and the last 5 genes have $\phi_l = 1.1$.
viii) The total computation user time was about 16 hours on a desktop with processor with the following specifications: Intel(R) Core(TM) i5-7600 CPU @ 3.50GHz, 3504 Mhz and Installed physical memory (RAM): 16.0 GB.

It shows that the bootstrap method based on pivotal quantities controls FWER under both complete and partial null hypotheses. This implies the proposed method controls FWER strongly, see Dudoit *et al.* [3]. Without adjustment of multiplicity, it is well known that the overall error rates often exceed the nominal level, particularly in large-scale tests.

Simultaneous tests based on large-sample approximation fail to control FWER in the strong sense in RNA sequencing data analysis. While the overall error rates are controlled at nominal level $\alpha = 0.05$, in average more than 85% of "real" misexpressed genes are detected as differentially expressed genes using the bootstrap method in Section 3.2. Note that it is not useful to address the power rates when the method does not control FWER.

To investigate the performance of the bootstrap method in estimation of quantiles, we generate $1,000$ samples as described above and obtain the $(1-\alpha)$-th quantile of the sampling distribution of pivotal quantities in (2.8). Since the quantiles are generated from a given underlying distribution of maximum modulus distribution empirically, it can be used as a benchmark to evaluate the performance of the proposed method. The results are summarized in Table 2.

Table 2: Quantiles q_α of detecting differentially expressed genes/isoforms — nominal type-1 error rate $\alpha = 0.05$.

ϕ_l	Simulation	MVN	Bootstrap
1.000	3.604	3.519 (0.090)	3.606 (0.094)
1.050 (1.1)	3.617	3.522 (0.086)	3.611 (0.094)
1.010	3.605	3.524 (0.090)	3.609 (0.095)
1.001	3.604	3.516 (0.084)	3.604 (0.097)

Notes:

i) Simulation size = 1,000. Bootstrap size $B = 200$.

ii) MVN denotes the method of large-sample approximation in Section 3.1 and the Algorithm in Section 4. The quantile is generated from $B = 200$ samples. We repeat the process for $1,000$ times. The mean value of these repeats is included outside of the parentheses and standard deviation is tabulated in the parentheses.

iii) "Bootstrap" means the parametric bootstrap method in Section 3.2. The quantile is generated from $B = 200$ bootstrap samples. We repeat the process for 1,000 times. The mean value of these repeats is included outside of the parentheses and standard deviation is tabulated in the parentheses.

iv) "Simulation" means: we generate observations from the model in (2.1) with the parameter value assigned in Section 4 and given underlying distributions for $1,000$ times; the upper α-th quantile of maximum modulus statistics based on pivotal quantiles in (2.8) is tabulated in the table.

v) The total computation user time was about 8 hours on a desktop with processor with the following specifications: Intel(R) Core(TM) i5-7600 CPU @ 3.50GHz, 3504 Mhz and Installed physical memory (RAM): 16.0 GB.

It shows from Table 2 that the bootstrap quantiles in Section 3.2 are closer to the simulated quantiles as compared to that generated from MVN. A closer examination sees the quantiles based on normal theory are generally below the simulated quantiles. Therefore, the large-sample approximation method provides a liberal estimation of FWER, as evidenced in Table 1.

5. CONCLUSION AND FUTURE WORK

In this article, we have proposed the parametric bootstrap method based on pivotal quantities in detecting differentially expressed genes for RNA-sequencing data. We have formulated the problem using the Poisson generalized linear models. We have derived the joint limiting distribution of the vector containing pivotal quantities. We have conducted an empirical study to show that the proposed method controls FWER and FDR strongly in detecting differentially expressed genes. The bootstrap method requires a large computation time, parallel computation is recommended particularly for large-scale inference. When data "apparently" violate Poisson distributional assumption, we will investigate the methods involving a large value of overdispersion. To capture the within genes' variation and between genes' variation, we will study the resampling methods, such as moving block bootstrap method in the future work.

6. SOFTWARE

We use the function `glm()` in `R` to obtain maximum likelihood estimation of the parameters in model (2.1). Note that computation of the estimation using `glm()` in `R` may encounter non-convergence. Alternatively, iterative weighted least squares method of Wedderburn [12] may be used in the estimation. Our experience in the simulation study (results not shown) shows that using 20-step iterative weighted least squares method provides satisfactory approximation of the overall Type-I error rates. We use the function `rmvnorm()` of Genz *et al.* [5] in `R` to generate multivariate normal random variables. We use the function `calcNormFactors()` of Chen *et al.* [2] to obtain the library size. Software in the form of `R` code is available on request from the author (bli@citadel.edu).

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VARIANCE ESTIMATION USING RANDOMIZED RESPONSE TECHNIQUE

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Abstract:

- Variance estimation is a well-studied topic in survey sampling but not much work has been done in this area in the context of Randomized Response Technique (RRT) models. We propose here some variance estimators for sensitive variables using auxiliary information. We examine the performance of the proposed estimators through a simulation study and through a numerical example.

Key-Words:

- *auxiliary information; Mean Square Error; Randomized Response Technique; respondent privacy; variance estimation.*

AMS Subject Classification:

- 62D05.

1. INTRODUCTION

When conducting surveys, it is sometimes difficult to make a direct observation on the variable of interest. This is more so in the case where the research involves a topic that is a taboo in nature. In surveys on such topics, some of the respondents might give false responses. To offer a solution to this, a Randomized Response Technique (RRT) was developed by Warner [7]. The technique allows respondents to provide a response while maintaining their privacy.

The problem of mean and variance estimation is a topic that has been explored very well by researchers, although less so the problem of variance estimation. This is particularly the case in the context of RRT models. This is the main focus of this study where we examine variance estimation of a sensitive study variable using a highly correlated but non-sensitive auxiliary variable. According to Collins *et al.* [1], the auxiliary variables when combined with the main study variable help to achieve more efficient estimators.

In this paper, three variance estimators have been proposed under RRT using one auxiliary variable and two scrambling variables. In Section 2, some of the variance estimators in literature are reviewed. In Section 3, we propose a new class of variance estimators under RRT and derive their Bias as well as their MSE. We provide a comparison of the proposed estimators in Section 4. A numerical study is conducted in Section 5 based on real data. Some concluding remarks are given in Section 6.

2. ESTIMATORS IN LITERATURE

Let a simple random sample of size n be extracted without replacement from a finite population $U = \{U_1, U_2, ..., U_N\}$. Let Y be a sensitive variable of interest and X be a positively correlated auxiliary variable. Let (x_i, y_i) be the observed (X, Y) values for the i-th population unit U_i. Let $(\bar{x}, \bar{y})$ and $(\bar{X}, \bar{Y})$ be the sample and population means, and (s_x^2, s_y^2) and (σ_x^2, σ_y^2) be the sample and population variances respectively. Let

$$s_y^2 = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2\,, \qquad s_x^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2\,,$$

$$\sigma_y^2 = \frac{1}{N-1}\sum_{i=1}^{N}(Y_i - \bar{Y})^2\,, \qquad \sigma_x^2 = \frac{1}{N-1}\sum_{i=1}^{N}(X_i - \bar{X})^2\,,$$

$$\bar{X} = \frac{1}{N}\sum_{i=1}^{N}X_i\,, \quad \bar{Y} = \frac{1}{N}\sum_{i=1}^{N}Y_i\,, \quad \bar{x} = \frac{1}{N}\sum_{i=1}^{N}x_i\,, \quad \bar{y} = \frac{1}{N}\sum_{i=1}^{N}y_i\,.$$

An unbiased estimator for the finite population variance is the sample variance given by:

$$t_0 = s_y^2\,.$$

Up to the first degree of approximation, its variance is given by

$$V(t_0) = \theta\sigma_y^4(\lambda_{40} - 1)\,,$$

where

$$\lambda_{rs} = \frac{\mu_{rs}}{\mu_{20}^{\frac{r}{2}}\,\mu_{02}^{\frac{s}{2}}}\,,\qquad \mu_{rs} = \frac{1}{N-1}\sum_{i=1}^{N}(Y_i - \bar{Y})^r\,(X_i - \bar{X})^s\,,\qquad \text{and}\qquad \theta = \frac{1}{n}\,.$$

Also 'r' and 's' are non-negative integers, μ_{20} and μ_{02} are the second order moments and λ_{rs} is the moment ratio.

Isaki [4] proposed the following ratio estimator of population variance using auxiliary information:

$$t_1 = s_y^2\left(\frac{\sigma_x^2}{s_x^2}\right).$$

The expressions for Bias and Mean Square Error (MSE) of the estimator, up to the first order of approximation, are given by

$$\text{B}(t_1) = \theta\sigma_y^2(\lambda_{04} - 1)\,[1 - f_{04}]$$

and

$$\text{MSE}(t_1) = \theta\sigma_y^4(\lambda_{40} - 1) + (\lambda_{04} - 1)\,[1 - 2f_{04}]\,,$$

where

$$f_{04} = \frac{(\lambda_{22} - 1)}{(\lambda_{04} - 1)}\,.$$

The regression estimator of population variance was also proposed by Isaki [4] as

$$t_2 = s_y^2 + \alpha(\sigma_x^2 - s_x^2)\,,\qquad \text{where}\quad \alpha = \left(\frac{\sigma_y^2}{\sigma_x^2}\right)f_{04}\,.$$

The MSE of t_2 is given by

$$\text{MSE}(t_2) = \theta\sigma_y^4(\lambda_{40} - 1)\,(1 - p^2)\,,\qquad \text{where}\quad p = (\lambda_{22} - 1)/\sqrt{(\lambda_{40} - 1)\,(\lambda_{04} - 1)}\,.$$

3. PROPOSED ESTIMATORS

Since Y is sensitive in nature, and hence subject to social desirability bias, we observe only a scrambled version of Y as given by Diana and Perri [2]. This is given by $Z = TY + S$, where T and S are scrambling variables. We also assume that Y, T and S are mutually uncorrelated. We also assume $E(S) = 0$ and $E(T) = 1$.

To obtain the Bias and MSE expressions for the proposed estimators, we define the following error terms:

$$s_z^2 = \sigma_z^2(1 + \delta_z)\qquad \text{and}\qquad \bar{z} = \bar{Z}(1 + e_z)\,,$$

where

$$\delta_z = \frac{s_z^2 - \sigma_z^2}{\sigma_z^2} \qquad \text{and} \qquad e_z = \frac{\bar{z} - \bar{Z}}{\bar{Z}}$$

such that

$$E(\delta_z) = E(e_z) = 0\,, \quad E(\delta_z^2) = \theta(\lambda_{40} - 1)\,, \quad \text{and} \quad E(e_z^2) = \theta C_z^2\,; \quad \text{and} \quad E(\delta_z e_z) = \theta \lambda_{30} C_z$$

where

$$C_z^2 = C_y^2 \sigma_T^2 + \left(\frac{\sigma_S^2}{\bar{Y}^2}\right).$$

We now propose several population variance estimators under RRT.

3.1. A basic variance estimator under RRT

Based on the RRT model $Z = TY + S$, we have σ_z^2 as

$$\begin{aligned}
\sigma_z^2 &= \sigma_{TY+S}^2 = \sigma_{TY}^2 + \sigma_S^2 \\
&= \Big(\sigma_T^2 * \sigma_Y^2 + \sigma_T^2 * \big(E[Y]\big)^2 + \big(E[T]\big)^2 * \sigma_Y^2\Big) + \sigma_S^2 \\
&= \Big(\sigma_T^2 * \sigma_Y^2 + \sigma_T^2 * (\mu_Y)^2 + \sigma_Y^2\Big) + \sigma_S^2 \\
&= \sigma_T^2 * \sigma_Y^2 + \sigma_T^2 * \mu_Y^2 + \sigma_Y^2 + \sigma_S^2\,.
\end{aligned}$$

Rearranging, we get

$$\sigma_y^2 = \frac{\sigma_z^2 - \sigma_S^2 - (\sigma_T^2 * \bar{Z}^2)}{\sigma_T^2 + 1}\,.$$

Estimating σ_z^2 by its unbiased estimator s_z^2, we have our first proposed estimator given by

$$t_0(R) = \frac{s_z^2 - \sigma_S^2 - \sigma_T^2 * \bar{z}^2}{\sigma_T^2 + 1}\,. \tag{3.1}$$

Rewriting (3.1), we have

$$t_0(R) = \frac{\sigma_z^2(1+\delta_z) - \sigma_S^2 - \sigma_T^2\big[\bar{Z}(1+e_z)\big]^2}{\sigma_T^2 + 1}\,.$$

Subtracting σ_y^2 on both sides, we obtain

$$\big(t_0(R) - \sigma_y^2\big) = \frac{\sigma_z^2\,\delta_z - 2\,\sigma_T^2\,\bar{Z}^2\,e_z - \sigma_T^2\,\bar{Z}^2\,e_z^2}{\sigma_T^2 + 1}\,. \tag{3.2}$$

By taking the expectation on both sides of (3.2), the Bias of $t_0(R)$ is obtained as

$$\text{Bias}\big(t_0(R)\big) = -\theta\left(\frac{\sigma_T^2\,\bar{Z}^2}{\sigma_T^2 + 1}\right) C_z^2\,.$$

By squaring both sides of (3.2) and using the first order approximation, the MSE is obtained as

$$\text{MSE}\big(t_0(R)\big) = \theta\left(\frac{1}{(\sigma_T^2 + 1)^2}\right)\Big(\sigma_z^4(\lambda_{40} - 1) + 4\,\sigma_T^4\,\bar{Z}^4 C_z^2 - 4\,\sigma_z^2\sigma_T^2\,\bar{Z}^2\lambda_{30}\,C_z\Big)\,. \tag{3.3}$$

3.2. The ratio estimator under RRT

Isaki [4] proposed the classical ratio estimator $t_1 = s_y^2\left(\frac{\sigma_x^2}{s_x^2}\right)$. The RRT version of t_1 is

$$t_1(R) \;=\; \frac{s_z^2 - \sigma_S^2 - \sigma_T^2 * \bar{z}^2}{\sigma_T^2 + 1} * \left(\frac{\sigma_x^2}{s_x^2}\right). \tag{3.4}$$

To obtain the Bias and MSE, we define the following error terms:

$$s_x^2 \;=\; \sigma_x^2(1+\delta_x), \qquad \text{where} \quad \delta_x = \frac{s_x^2 - \sigma_x^2}{\sigma_x^2}\,,$$

such that

$$E(\delta_x) = 0\,, \qquad E(\delta_x^2) = \theta(\lambda_{04} - 1) \qquad \text{and} \qquad E(\delta_x e_z) = \theta\lambda_{12} C_z\,.$$

Rewriting (3.4), we have

$$t_1(R) \;=\; \frac{\sigma_z^2 - \sigma_S^2 - \sigma_T^2\bar{Z}^2}{\sigma_T^2+1} + \frac{2\,\sigma_T^2\bar{Z}^2 e_z\delta_x - \sigma_z^2\delta_z\delta_x - \sigma_T^2\bar{Z}^2 e_z^2}{\sigma_T^2+1}\,.$$

Subtracting σ_y^2 and taking the expectation on both sides, the Bias of $t_1(R)$ is obtained as

$$\mathrm{Bias}\big(t_1(R)\big) \;=\; \theta\left(\frac{2\,\sigma_T^2\bar{Z}^2\lambda_{12}C_z - \sigma_z^2(\lambda_{22}-1) - \sigma_T^2\bar{Z}^2 C_z^2}{\sigma_T^2+1}\right). \tag{3.5}$$

For MSE, we have

$$\begin{aligned} t_1(R) \;=\; &\frac{\sigma_z^2 + \sigma_z^2\delta_z - \sigma_S^2 - \sigma_T^2\bar{Z}^2 - 2\,\sigma_T^2\bar{Z}^2 e_z - \sigma_T^2\bar{Z}^2 e_z^2}{\sigma_T^2+1} \\ &\frac{-\sigma_z^2\delta_x - \sigma_z^2\delta_z\delta_x + \sigma_S^2\delta_x + \sigma_T^2\bar{Z}^2\delta_x + 2\,\sigma_T^2\bar{Z}^2 e_z\delta_x + \sigma_T^2\bar{Z}^2 e_z^2\delta_x}{\sigma_T^2+1}\,. \end{aligned}$$

Simplifying and ignoring second and higher order terms,

$$t_1(R) \;=\; \frac{\sigma_z^2 - \sigma_S^2 W - \sigma_T^2\bar{Z}^2}{\sigma_T^2+1} + \frac{\sigma_z^2\delta_z - 2\,\sigma_T^2\bar{Z}^2 e_z - \sigma_z^2\delta_x + \sigma_S^2\delta_x + \sigma_T^2\bar{Z}^2\delta_x}{\sigma_T^2+1}\,.$$

Squaring and taking the expectation on both sides, we have

$$\mathrm{MSE}\big(t_1(R)\big) \;=\; E\left(\frac{\sigma_z^2\delta_z}{\sigma_T^2+1} - \frac{2\,\sigma_T^2\bar{Z}^2 e_z}{\sigma_T^2+1} - \sigma_y^2\delta_x\right)^2.$$

After some simplifications, the MSE of $t_1(R)$ is obtained as

$$\begin{aligned} \mathrm{MSE}\big(t_1(R)\big) \;=\; \theta\frac{1}{(\sigma_T^2\!+\!1)^2}\bigg[&\sigma_z^4(\lambda_{40}\!-\!1) - 2\,\sigma_z^2\sigma_y^2(\lambda_{22}\!-\!1)\,(\sigma_T^2\!+\!1) + \sigma_y^4(\lambda_{04}\!-\!1)\,(\sigma_T^2\!+\!1)^2 \\ &+\; 4C_z\Big(\sigma_T^4\bar{Z}^4 C_z - \sigma_z^2\sigma_T^2\bar{Z}^2\lambda_{30} + \sigma_T^2\sigma_y^2\bar{Z}^2\lambda_{12}(\sigma_T^2+1)\Big)\bigg]. \end{aligned} \tag{3.6}$$

3.3. A generalized variance estimator under RRT

We now propose the following class of generalized population variance estimators:

$$t_p(R) \;=\; \left[\left(\left(\frac{s_z^2-\sigma_S^2-\sigma_T^2 * \bar{z}^2}{\sigma_T^2+1}\right)+(\sigma_x^2-s_x^2)\right) * \left(\frac{(\alpha\sigma_x^2+\beta)}{\omega(\alpha s_x^2+\beta)+(1-\omega)\,(\alpha\sigma_x^2+\beta)}\right)^g\right], \tag{3.7}$$

where g, α, β and ω are suitably chosen constants. We would choose $g=1$ for positive correlation between Y and X, and -1 for negative correlation. α and β are known parameters associated with the auxiliary variable and ω is obtained from optimality consideration.

Using Taylor series approximation, we obtain the bias of the generalized estimator $t_p(R)$ as

$$\operatorname{Bias}\big(t_p(R)\big) \;=\; \frac{-\theta\,\sigma_T^2\,\bar{Z}^2}{\sigma_T^2+1}\,C_z^2-(g\,\omega\,\psi_i)\,\theta\left(\frac{\sigma_z^2(\lambda_{22}-1)-2\,\sigma_T^2\,\bar{Z}^2\lambda_{12}C_z}{\sigma_T^2+1}-\sigma_x^2(\lambda_{04}-1)\right), \tag{3.8}$$

where $\psi_i=\frac{\alpha\sigma_x^2}{\alpha\sigma_x^2+\beta}$.

The mean square error is given by

$$\begin{aligned}\operatorname{MSE}\big(t_p(R)\big) \;=\; \theta\Bigg[&\left(\frac{\sigma_z^4(\lambda_{40}-1)+4\,\sigma_T^4\,\bar{Z}^4C_z^2-4\,\sigma_z^2\sigma_T^2\,\bar{Z}^2\lambda_{30}C_z}{(\sigma_T^2+1)^2}\right)\\ &+\left((\sigma_x^2+Q\,\sigma_y^2)^2\,(\lambda_{04}-1)\right)\\ &-2\left(\frac{\sigma_z^2(\lambda_{22}-1)-2\,\sigma_T^2\,\bar{Z}^2\lambda_{12}C_z}{\sigma_T^2+1}\right)(\sigma_x^2+Q\,\sigma_y^2)\Bigg],\end{aligned} \tag{3.9}$$

where $Q=g\,\omega\,\psi_i$.

Differentiate (3.9) w.r.t Q:

$$2\,\sigma_y^2(\sigma_x^2+Q\,\sigma_y^2)\,(\lambda_{04}-1) \;=\; 2\,\sigma_y^2\left(\frac{\sigma_z^2(\lambda_{22}-1)-2\,\sigma_T^2\,\bar{Z}^2\lambda_{12}C_z}{\sigma_T^2+1}\right),$$

$$Q_{\text{opt}} \;=\; \frac{1}{\sigma_y^2}\left[\left(\frac{\sigma_z^2(\lambda_{22}-1)-2\,\sigma_T^2\,\bar{Z}^2\lambda_{12}C_z}{\sigma_T^2+1}\right)\left(\frac{1}{(\lambda_{04}-1)}\right)-\sigma_x^2\right].$$

The MSE at this optimum value is given by

$$\begin{aligned}\operatorname{MSE}\big(t_p(R)\big)_{\text{opt}} \;=\; \frac{\theta}{(\sigma_T^2+1)^2}\Bigg[&\left(\sigma_z^4(\lambda_{40}-1)+4\,\sigma_T^4\,\bar{Z}^4C_z^2-4\,\sigma_z^2\sigma_T^2\,\bar{Z}^2\lambda_{30}C_z\right)\\ &-\frac{1}{(\lambda_{04}-1)}\left(\sigma_z^2(\lambda_{22}-1)-2\,\sigma_T^2\,\bar{Z}^2\lambda_{12}C_z\right)^2\Bigg].\end{aligned} \tag{3.10}$$

4. SIMULATION STUDY

In this section, we use a simulation study to evaluate how efficient the generalized estimator $t_p(R)$ is as compared to both the basic estimator $t_0(R)$ and the ratio estimator $t_1(R)$. We first consider samples of size $N = 1000$ each from three bivariate normal populations determined by the following means and covariance matrices:

$$\begin{aligned}
&\text{Population I:} && \mu = \begin{bmatrix} 6 \\ 4 \end{bmatrix}, \quad \Sigma = \begin{bmatrix} 4 & 1.6 \\ 1.6 & 1 \end{bmatrix}, && \rho_{yx} = 0.80\,; \\
&\text{Population II:} && \mu = \begin{bmatrix} 6 \\ 4 \end{bmatrix}, \quad \Sigma = \begin{bmatrix} 4 & 2.25 \\ 2.25 & 2 \end{bmatrix}, && \rho_{yx} = 0.80\,; \\
&\text{Population III:} && \mu = \begin{bmatrix} 6 \\ 4 \end{bmatrix}, \quad \Sigma = \begin{bmatrix} 4 & 1.2 \\ 1.2 & 1 \end{bmatrix}, && \rho_{yx} = 0.60\,.
\end{aligned} \tag{4.1}$$

These 1000 observations are treated as our finite populations. For the 1000 values generated from these distributions, the means, variances, covariances, and correlations are given by

$$\begin{aligned}
&\text{Population I:} && \mu_x = 6.029, \quad \mu_y = 4.007, \quad \sigma_x^2 = 3.8862, \quad \sigma_y^2 = 0.9450, \\
& && \sigma_{xy} = 1.5284, \quad \rho_{yx} = 0.7975389\,; \\
&\text{Population II:} && \mu_x = 6.021, \quad \mu_y = 3.9836, \quad \sigma_x^2 = 3.9467, \quad \sigma_y^2 = 1.9998, \\
& && \sigma_{xy} = 2.2382, \quad \rho_{yx} = 0.7967094\,; \\
&\text{Population III:} && \mu_x = 5.962, \quad \mu_y = 3.971, \quad \sigma_x^2 = 4.1149, \quad \sigma_y^2 = 0.9560, \\
& && \sigma_{xy} = 1.2442, \quad \rho_{yx} = 0.5927674\,.
\end{aligned}$$

For each population, we consider samples of sizes 200 and 500. The scrambling variables S and T are assumed to have normal distributions with $E(S) = 0$ and $E(T) = 1$. We have used different values for $\mathrm{Var}(S)$ and $\mathrm{Var}(T)$.

Before presenting the simulation results, we would like to note that in most studies, researchers have compared estimators only with respect to the *Percent Relative Efficiency* which is defined as

$$\mathrm{PRE} = \frac{\mathrm{MSE}\big(t_0(R)\big)}{\mathrm{MSE}\big(t_i(R)\big)} \times 100, \qquad \text{where} \quad i = 0, 1 \text{ and } p\,.$$

However, for estimators based on RRT methodology, one needs to also consider the *Privacy Protection* offered by the RRT model. With that in mind, Gupta *et al.* [3] introduced a unified measure of estimator quality (δ) given by

$$\delta = \frac{\text{Theoretical MSE}}{\Delta_{DP}}, \qquad \text{where} \quad \Delta_{DP} = E(Z-Y)^2 = \sigma_T^2(\mu_y^2 + \sigma_y^2) + \sigma_s^2$$

is the privacy level for the model $Z = TY + S$, as per Yan *et al.* [8]. A smaller value of (δ) is to be preferred. Khalil *et al.* [6] used this unified measure to compare the performance of various mean estimators under RRT.

Table 1: Theoretical (**bold**) and empirical MSEs and PREs of the estimators for Population I with $\sigma_T^2 = 0.5$, $\sigma_y^2 = 1$ and $\rho_{yx} = 0.80$.

Var(S)	n	**Estimator**	**Mean($\widehat{\sigma}_y^2$)**	**MSE**	**PRE**	δ
0.2	200	$t_0(R)$	1.018416	**0.4593715** 0.4629093	**100** 100	0.052801
		$t_1(R)$	0.9873038	**0.4166811** 0.4137594	**110.2453** 111.8788	0.04789438
		$t_p(R)$	0.9708478	**0.3685766** 0.3689481	**124.6339** 125.4673	0.04236513
	500	$t_0(R)$	1.021572	**0.1995375** 0.2100302	**100** 100	0.02293534
		$t_1(R)$	0.9846944	**0.1430092** 0.146612	**139.5277** 143.2558	0.01643784
		$t_p(R)$	0.9999683	**0.0946721** 0.0957580	**210.7669** 219.3343	0.01088185
0.5	200	$t_0(R)$	1.034554	**0.5512713** 0.5593184	**100** 100	0.06125237
		$t_1(R)$	0.9986482	**0.4943552** 0.5045654	**111.5131** 110.8515	0.05492836
		$t_p(R)$	0.9854447	**0.4320352** 0.4187965	**127.5987** 133.5537	0.04800391
	500	$t_0(R)$	1.023019	**0.2022691** 0.1991505	**100** 100	0.02247434
		$t_1(R)$	0.9816713	**0.1866725** 0.182478	**108.3550** 109.1367	0.02074139
		$t_p(R)$	1.00232	**0.1686173** 0.1685935	**119.9575** 118.1246	0.01873526
1	200	$t_0(R)$	1.032376	**0.6313128** 0.6288249	**100** 100	0.06645398
		$t_1(R)$	0.9967019	**0.5716984** 0.5582806	**110.4275** 112.6359	0.06017878
		$t_p(R)$	0.9682892	**0.494106** 0.5058227	**127.7686** 124.3172	0.05201116
	500	$t_0(R)$	1.040029	**0.2705931** 0.2652877	**100** 100	0.02848348
		$t_1(R)$	0.9968461	**0.212635** 0.2254085	**127.2570** 117.6919	0.02238263
		$t_p(R)$	0.9791635	**0.1965888** 0.204013	**137.6442** 130.0347	0.02069356

Tables 1, 2 and 3 show the values of the theoretical MSEs and empirical MSEs. The values from the table confirm that the basic estimator $t_0(R)$ and the ratio estimator $t_1(R)$ are less efficient as compared to the generalized estimator $t_p(R)$. Also, while comparing the generalized estimator $t_p(R)$ with the ratio estimator $t_1(R)$ and basic estimator $t_0(R)$, we note that as the variance of T or variance of S increase, the MSEs increase. This is expected since adding more noise makes the MSE increase. However, if we look at the unified measure (δ), we find that it does not always increase as variance of T or variance of S increase, or at least not to the same extent as does the MSE. For example, for the generalized estimator

$t_p(R)$, theoretical MSE for Population II, with sample size 500, is 0.09227229 for $\sigma_T^2 = 0.2$ but increases to 0.3790013 for $\sigma_T^2 = 1$. In contrast, the (δ) value decreases from 0.023659 to 0.020499. Admittedly, this is not a big drop in (δ) value but at least it is not going up. The important point here is that the 310% increase in MSE (from 0.09227229 to 0.3790013) is more than offset by the significant increase in privacy level in using $\sigma_T^2 = 1$ as compared to $\sigma_T^2 = 0.2$. In another example, for the generalized estimator $t_p(R)$, theoretical MSE for Population III, with sample size 500, is 0.1877209 for $\sigma_T^2 = 0.5$ but increases to 0.3634541 for $\sigma_T^2 = 1$. In contrast, the (δ) value decreases from 0.021453 to 0.021069.

Table 2: Theoretical (**bold**) and empirical MSEs and PREs of the estimators for Population II with $\sigma_s^2 = 0.5$, $\sigma_y^2 = 2$ and $\rho_{yx} = 0.80$.

Var(T)	n	**Estimator**	**Mean($\widehat{\sigma}_y^2$)**	**MSE**	**PRE**	δ
0.2	200	$t_0(R)$	1.961504	**0.3353948** 0.3330506	**100** 100	0.085998
		$t_1(R)$	1.938223	**0.3086746** 0.310405	**108.6564** 107.2955	0.079147
		$t_p(R)$	1.97547	**0.2604031** 0.2696629	**128.7983** 123.5062	0.066770
	500	$t_0(R)$	1.984015	**0.1299197** 0.1273284	**100** 100	0.033312
		$t_1(R)$	1.999045	**0.1057879** 0.1067183	**122.8114** 119.3126	0.027125
		$t_p(R)$	1.985764	**0.09227229** 0.09218931	**140.8003** 138.1162	0.023659
0.5	200	$t_0(R)$	1.997112	**0.8036853** 0.7958328	**100** 100	0.084651
		$t_1(R)$	1.988183	**0.7195406** 0.694571	**111.6942** 114.5790	0.075788
		$t_p(R)$	1.98627	**0.624445** 0.6421061	**128.7039** 123.9410	0.065772
	500	$t_0(R)$	1.991561	**0.2858802** 0.2751116	**100** 100	0.030111
		$t_1(R)$	1.982515	**0.2471334** 0.232594	**115.6784** 118.2797	0.026030
		$t_p(R)$	1.968053	**0.1816638** 0.1885275	**157.3677** 145.9265	0.019134
1	200	$t_0(R)$	1.981875	**1.170947** 1.167372	**100** 100	0.063335
		$t_1(R)$	2.002721	**1.014171** 0.5582806	**115.4585** 112.8290	0.054855
		$t_p(R)$	1.988997	**0.955732** 0.969496	**122.5183** 120.4101	0.051694
	500	$t_0(R)$	1.979819	**0.5567679** 0.531363	**100** 100	0.030114
		$t_1(R)$	1.998328	**0.4837988** 0.4790216	**115.0825** 110.9267	0.026168
		$t_p(R)$	1.971607	**0.3790013** 0.3843118	**146.9039** 138.2635	0.020499

Table 3: Theoretical (**bold**) and empirical MSEs and PREs of the estimators for Population III with $\sigma_s^2 = 0.25$, $\sigma_y^2 = 1$ and $\rho_{yx} = 0.60$.

Var(T)	n	**Estimator**	**Mean($\hat{\sigma}_y^2$)**	**MSE**	**PRE**	δ
0.2	200	$t_0(R)$	1.021512	**0.2249759** 0.223441	**100** 100	0.061637
		$t_1(R)$	1.037037	**0.1962207** 0.1958733	**114.6545** 114.0742	0.053759
		$t_p(R)$	0.979563	**0.1733191** 0.1752187	**129.8044** 127.5212	0.047484
	500	$t_0(R)$	0.99568	**0.09192312** 0.09384772	**100** 100	0.025184
		$t_1(R)$	1.035195	**0.08558669** 0.08575554	**107.4035** 109.4363	0.023448
		$t_p(R)$	0.995747	**0.06216159** 0.06279393	**147.8776** 149.4534	0.017030
0.5	200	$t_0(R)$	0.9830188	**0.6333537** 0.6304459	**100** 100	0.072383
		$t_1(R)$	1.039288	**0.5491218** 0.5699384	**115.3393** 110.6164	0.062756
		$t_p(R)$	0.971143	**0.4907475** 0.5044131	**129.0589** 124.9860	0.056085
	500	$t_0(R)$	0.9941702	**0.2469968** 0.2442127	**100** 100	0.028228
		$t_1(R)$	0.9846135	**0.2070803** 0.2115374	**119.2758** 115.4465	0.023666
		$t_p(R)$	0.9992722	**0.1877209** 0.1827657	**131.5766** 133.6206	0.021453
1	200	$t_0(R)$	0.9571123	**1.166476** 1.148805	**100** 100	0.067621
		$t_1(R)$	0.9954355	**1.092394** 1.087534	**106.7816** 105.6339	0.063327
		$t_p(R)$	0.9794743	**0.9463649** 0.9256485	**123.2585** 124.1081	0.054861
	500	$t_0(R)$	1.009706	**0.5152219** 0.4923866	**100** 100	0.029867
		$t_1(R)$	0.9918212	**0.4304643** 0.458314	**119.6898** 107.4343	0.024954
		$t_p(R)$	0.9856029	**0.3634541** 0.3569531	**141.7570** 137.9415	0.021069

5. APPLICATION

In this section, we use a real data to show the performance of the generalized estimator $t_p(R)$ in comparison to other estimators. For this data which can be obtained from James *et al.* [5], the population size is ($N = 777$). The study variable Y is the reported percent of alumni who donate. The auxiliary variable X is the student to faculty ratio. The scrambling variable S is taken to be a normal random variable with mean equal to zero and variance equal to 0.5. The scrambling variable T is taken to be a normal random variable with mean equal to 1 and variance equal to 0.2, 0.5, and 1.

Population Characteristics are given by

$$N = 777\,, \quad n = 200\,, \quad \mu_X = 14.08\,, \quad \mu_Y = 22.74\,,$$
$$\sigma_X = 3.95\,, \quad \sigma_Y = 12.39\,, \quad \sigma_{XY} = 19.7641\,, \quad \rho_{yx} = 0.40\,.$$

From the Table 4, it can be observed that the generalized estimator $t_p(R)$ performs better than the other estimators $t_0(R)$ and $t_1(R)$. Also, we can observe that the unified measure (δ) does not always increase as variance of T increases, or at least not to the same extent as does the MSE. For example, for the generalized estimator $t_p(R)$, theoretical MSE is 301.0716 for $\sigma_T^2 = 0.2$ but increases to 1196.559 for $\sigma_T^2 = 1$. In contrast, the (δ) value decreases from 2.23565474 to 1.78234135.

Table 4: Theoretical (**bold**) and empirical MSEs and PREs of the estimators.

n	Var(T)	Estimator	MSE	PRE	δ
500	0.2	$t_0(R)$	**519.1796** 490.2126	**100** 100	3.85525016
		$t_1(R)$	**435.4705** 437.4432	**119.2226** 112.0631	3.23365501
		$t_p(R)$	**301.0716** 297.7625	**172.4438** 164.6320	2.23565474
	0.5	$t_0(R)$	**896.6322** 888.2846	**100** 100	2.66917897
		$t_1(R)$	**643.4997** 620.5305	**139.3368** 143.1492	1.91563036
		$t_p(R)$	**596.1386** 570.0859	**150.4066** 155.8159	1.77464139
	1	$t_0(R)$	**1805.427** 1876.467	**100** 100	2.68928418
		$t_1(R)$	**1618.569** 1650.915	**111.5446** 113.6622	2.41094877
		$t_p(R)$	**1196.559** 1105.511	**150.8849** 169.7375	1.78234135

6. CONCLUSION

We propose here some variance estimators under RRT. These are the basic estimator $t_0(R)$, ratio estimator $t_1(R)$ and the generalized estimator $t_p(R)$. The simulation study reveals that the generalized estimator $t_p(R)$ is more efficient than the other estimators $t_0(R)$ and $t_1(R)$. We also examine the efficiency of the estimators relative to not just the MSE values, but also with respect to the unified measure of estimators quality (δ) and observe that while MSE always increases as the noise level increases, the (δ) value does not necessary follow this pattern. This highlights the significance of respondent under privacy.

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ON ARNOLD–VILLASEÑOR CONJECTURES FOR CHARACTERIZING EXPONENTIAL DISTRIBUTION BASED ON SAMPLE OF SIZE THREE

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Abstract:

- Arnold and Villaseñor [4] obtain a series of characterizations of the exponential distribution based on random samples of size two. These results were already applied in constructing goodness-of-fit tests in [7]. Extending the techniques from [4], we prove some of Arnold and Villaseñor's conjectures for samples of size three. An example with simulated data is discussed.

Key-Words:

- *exponential distribution; characterizations; order statistics.*

AMS Subject Classification:

- 62G30, 62E10.

1. INTRODUCTION

In general, the problem of characterization of probability distributions is described as follows. Suppose a family of distributions $\mathcal{F}$ possesses a property $\mathcal{A}$. If, conversely, a distribution has property $\mathcal{A}$ only if it is a member of that family, then property $\mathcal{A}$ characterizes the family $\mathcal{F}$. This result is referred to as a characterization of the distributions in $\mathcal{F}$. Primary motivation for characterizations problems is due to statistical applications. If a statistical procedure assumes that property $\mathcal{A}$ holds, then the underlying distribution must be a member of the family $\mathcal{F}$. Naturally, first characterizations results are for the normal family of distributions. The exponential distribution is one of the non-normal distributions, which has received a lot of attention as well. Comprehensive surveys of exponential characterizations can be found in [1], [3], [5], [6], and [8].

More recently, Arnold and Villaseñor [4] obtained a series of characterizations of the exponential distribution based on random samples of size two and conjectured possible generalizations for samples of size three. They provide motivation for their results by pointing out an example of a goodness-of-fit construction. A test for exponentiality based on the characterizations in [4] was recently constructed in [7]. Another possible use of the results in [4] and their generalizations, is in verifying modeling assumptions and in simulations (see also [8]). Extending the techniques from [4], we will prove some of Arnold and Villaseñor's conjectures.

Assume throughout that X_1, X_2, and X_3 are independent random variables with a common absolutely continuous cumulative distribution function (cdf) F, such that $F(0) = 0$ and probability density function (pdf) f. Denote $X_{2:2} := \max\{X_1, X_2\}$, $X_{3:3} := \max\{X_1, X_2, X_3\}$, and $\bar{F} = 1 - F$. Consider the relations:

$$\sum_{j=1}^{3} \frac{1}{j} X_j \quad \text{has pdf} \quad \sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} j\, f(j\,x)\,, \tag{1.1}$$

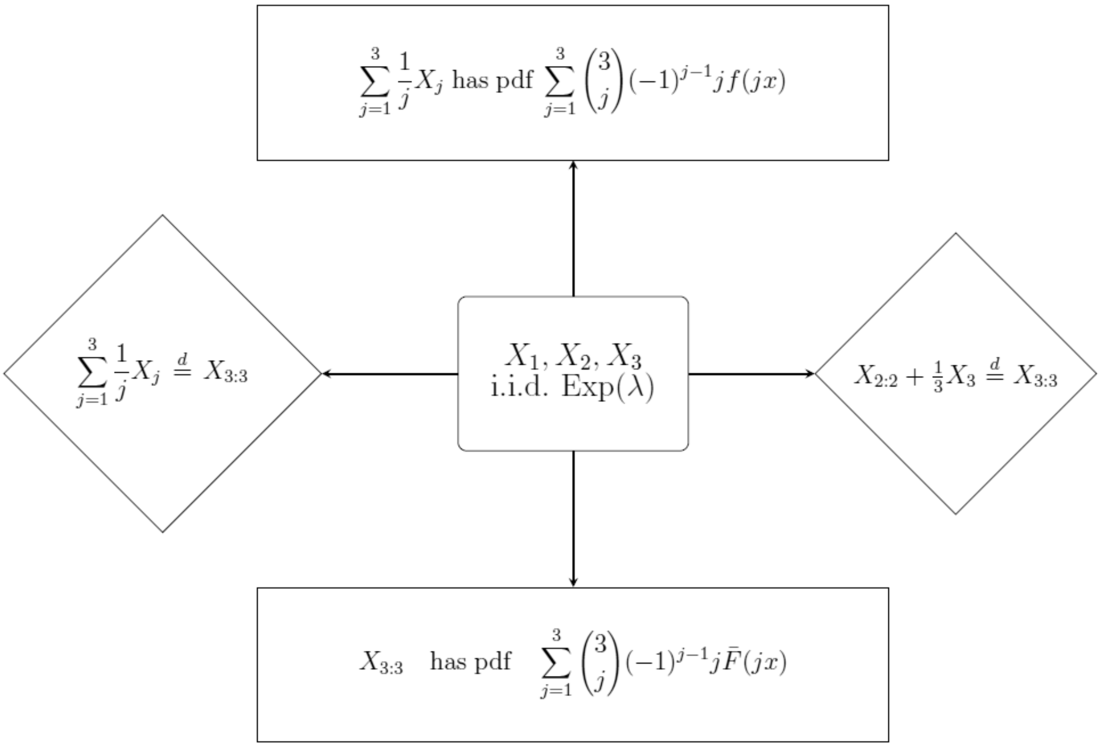
$$X_{3:3} \quad \text{has pdf} \quad \sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} j\, \bar{F}(j\,x)\,, \tag{1.2}$$

$$\sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} j\, f(jx) = \sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} j\, \bar{F}(j\,x)\,, \tag{1.3}$$

$$X_{2:2} + \frac{1}{3} X_3 \overset{d}{=} X_{3:3} \qquad \text{and} \qquad \sum_{j=1}^{3} \frac{1}{j} X_j \overset{d}{=} X_{3:3}\,, \tag{1.4}$$

where $\overset{d}{=}$ denotes equality in distribution. We will prove, under some regularity assumptions on F, that each one of these five conditions, on its own, is sufficient for X_1, X_2, and X_3 to be exponentially distributed.

We organize this paper as follows. Using Laplace transforms, in Section 2 we prove the characterization (1.1). In Section 3, we establish characterization (1.2) utilizing the Taylor series expansion of the cdf F. In Section 4, using a recurrent relation, we prove that (1.3) is a sufficient condition for having exponential parent. Section 5 contains characterization results based on (1.4). In Section 6 we provide an example with simulated data. In the concluding section, we discuss possible extensions of the given results.


$\sum_{j=1}^{3} \frac{1}{j} X_j$ has pdf $\sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} j f(jx)$
$\sum_{j=1}^{3} \frac{1}{j} X_j \overset{d}{=} X_{3:3}$
X_1, X_2, X_3
i.i.d. Exp(λ)
$X_{2:2} + \frac{1}{3} X_3 \overset{d}{=} X_{3:3}$
$X_{3:3}$ has pdf $\sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} j \bar{F}(jx)$

2. SUM OF THREE INDEPENDENT VARIABLES

To prove that (1.1) characterizes the exponential distribution, we will convert it into an equation for the Laplace transform $\varphi(t) := E[e^{-tX_1}]$.

Theorem 2.1. *Assume $\varphi(t)$ is finite for all t in a neighbourhood of zero. If for $x > 0$*

$$\sum_{j=1}^{3} \frac{1}{j} X_j \quad \textit{has pdf} \quad \sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} j\, f(j\, x)\,, \tag{2.1}$$

then $X_1 \sim \exp(\lambda)$ for some $\lambda > 0$.

Proof: It follows by (2.1), interchanging the order of summation and integration, that

$$\begin{aligned} \varphi(t)\ \varphi\left(\frac{t}{2}\right) \varphi\left(\frac{t}{3}\right) &= E\left[e^{-t\sum_{j=1}^{3} \frac{1}{j} X_j}\right] \\ &= \int_0^\infty e^{-tx} \left(\sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} j\, f(j\, x) \right) dx \\ &= \sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} \int_0^\infty e^{-tx} j\, f(j\, x)\, dx \\ &= \sum_{j=1}^{3} \binom{3}{j} (-1)^{j-1} \varphi\left(\frac{t}{j}\right). \end{aligned} \tag{2.2}$$

Dividing both sides of (2.2) by $\varphi(t)\,\varphi(t/2)\,\varphi(t/3)$, we obtain

$$1 \;=\; \alpha(t)\,\alpha\left(\frac{t}{2}\right) - 3\,\alpha(t)\,\alpha\left(\frac{t}{3}\right) + 3\,\alpha\left(\frac{t}{2}\right)\alpha\left(\frac{t}{3}\right), \tag{2.3}$$

where for $t > 0$

$$\alpha(t) := \frac{1}{\varphi(t)} = \sum_{k=0}^{\infty} a_k\, t^k\,. \tag{2.4}$$

Note that, the series in (2.4) is convergent in a neighbourhood of zero, by assumption. To prove the theorem, it is sufficient to show that

$$\alpha(t) = 1 + \lambda t\,, \qquad \lambda > 0\,. \tag{2.5}$$

We will prove (2.5) by calculating the coefficients of the series in (2.4) to be: $a_0 = 1$, $a_1 = \lambda > 0$, and $a_k = 0$ for $k \geq 2$. It is clear that $a_0 = \varphi^{-1}(0) = 1$. Applying Cauchy formula for multiplication of two power series, we have for any nonzeros p and q,

$$\alpha\left(\frac{t}{p}\right)\alpha\left(\frac{t}{q}\right) = \sum_{k=0}^{\infty}\left(\sum_{j=0}^{k} \frac{1}{p^j\, q^{k-j}}\; a_j\, a_{k-j}\right) t^k\,. \tag{2.6}$$

Now, (2.3) and (2.6) yield for $k \geq 1$

$$\sum_{j=0}^{k}\left(\frac{1}{2^{k-j}} - \frac{3}{3^{k-j}} + \frac{3}{2^j\, 3^{k-j}}\right) a_j\, a_{k-j} \;=\; 0\,. \tag{2.7}$$

Setting $k = 1$ we see that equation (2.7) has as solution any a_1. The assumption $F(0) = 0$ implies that there is $\lambda > 0$, such that $a_1 = \lambda > 0$. If $k = 2$, then (2.7) yields $a_2 = 0$. Assuming $a_j = 0$ for $2 \leq j \leq k-1$, it follows from (2.7) that

$$\left(1 - \frac{1}{2^{k-1}}\right) a_k \;=\; 0\,.$$

Thus, $a_k = 0$ for any $k \geq 3$. Therefore, (2.5) holds, which completes the proof. □

Note that, conversely, if $X_i \sim \exp(\lambda)$ for $i = 1, 2, 3$, then (2.1) holds true. To show this, it is sufficient to verify (2.2). Indeed, assuming $X_1 \sim \exp(\lambda)$, we have $\varphi(t) = (1 + \lambda t)^{-1}$. Therefore,

$$\begin{aligned}
\int_0^\infty e^{-tx}\left(\sum_{j=1}^{3}\binom{3}{j}(-1)^{j-1} j\, f(jx)\right) dx \;&=\; 3\,\varphi(t) - 3\,\varphi\left(\frac{t}{2}\right) + \varphi\left(\frac{t}{3}\right)\\
&=\; \frac{3}{1+\lambda t} - \frac{6}{2+\lambda t} + \frac{3}{3+\lambda t}\\
&=\; \varphi(t)\,\varphi\left(\frac{t}{2}\right)\varphi\left(\frac{t}{3}\right)\\
&=\; E\left[e^{-t\left(X_1 + \frac{1}{2}X_2 + \frac{1}{3}X_3\right)}\right],
\end{aligned}$$

which is equivalent to (2.1).

3. MAXIMUM OF THREE INDEPENDENT VARIABLES

In this section we will prove that, under some regularity assumptions on F, condition (1.2) is sufficient for X_1, X_2, and X_3 to be exponentially distributed. The proof will be based on the Taylor series expansion of F.

Theorem 3.1. *Assume the cdf F has a power series representation for x in a neighborhood of zero. If for $x > 0$*

$$X_{3:3} \quad \textit{has pdf} \quad \sum_{k=1}^{3} \binom{3}{k} (-1)^{k-1} k\,\bar{F}(kx)\,, \tag{3.1}$$

then $X_1 \sim \exp(1)$.

Proof: The relation (3.1) implies

$$F^2(x)\,f(x) + F(x) - 2\,F(2x) + F(3x) \;=\; 0\,. \tag{3.2}$$

Since $F(x) = \sum_{k=0}^{\infty} c_k x^k$ and $f(x) = \sum_{k=0}^{\infty} (k+1)\,c_{k+1} x^k$, Cauchy formula for the product of three power series yields

$$F^2(x)\,f(x) \;=\; \sum_{k=0}^{\infty} \left[\sum_{i=0}^{k} \sum_{j=0}^{i} c_j\,c_{i-j}\,(k+1-i)\,c_{k+1-i} \right] x^k\,. \tag{3.3}$$

Using (3.2) and (3.3), we obtain for any $k \geq 0$

$$\sum_{i=0}^{k} \sum_{j=0}^{i} c_j\,c_{i-j}\,(k+1-i)\,c_{k+1-i} + c_k(1 - 2^{k+1} + 3^k) \;=\; 0\,. \tag{3.4}$$

Since $F(0) = 0$, we have $c_0 = 0$. Also (3.4) with $k = 1$ yields $c_0^2 c_1 = 0$, which in turn implies that c_1 is undetermined. Let us set $c_1 = \delta$, where $-\infty < \delta < \infty$. Equation (3.4) with $k = 2$ yields $c_1^3 + 2\,c_2 = 0$. Hence, $c_2 = \delta^3/2$. We will prove by induction that

$$c_k = (-1)^{k-1} \frac{\delta^{2k-1}}{k!}\,, \qquad k = 1, 2, 3, \ldots\,. \tag{3.5}$$

Indeed, assuming (3.5) holds true for $1, 2, \ldots, k$, we have

$$\sum_{i=0}^{k+1} \sum_{j=0}^{i} c_j\,c_{i-j}\,(k+2-i)\,c_{k+2-i} \;=\; \sum_{i=2}^{k+1} \sum_{j=1}^{i-1} \frac{(-1)^{k+1}\,\delta^{2k+1}}{j!\,(i-j)!\,(k+1-i)!}\,. \tag{3.6}$$

Observe that

$$\begin{aligned} \sum_{i=2}^{k+1} \sum_{j=1}^{i-1} \frac{1}{j!\,(i-j)!\,(k+1-i)!} &= \sum_{i=2}^{k+1} \frac{1}{i!\,(k+1-i)!} \sum_{j=1}^{i-1} \frac{i!}{j!\,(i-j)!} \\ &= \frac{1}{(k+1)!} \sum_{i=2}^{k+1} \frac{(k+1)!}{i!\,(k+1-i)!}\,(2^i - 2) \\ &= \frac{1}{(k+1)!} \left[\sum_{i=2}^{k+1} \binom{k+1}{i} 2^i - 2 \sum_{i=2}^{k+1} \binom{k+1}{i} \right] \\ &= \frac{1}{(k+1)!} \left(3^{k+1} - 2^{k+2} + 1 \right). \end{aligned} \tag{3.7}$$

It follows from (3.4), (3.6) and (3.7) that

$$(-1)^{k+1}\frac{\delta^{2k+1}}{(k+1)!}\left(3^{k+1}-2^{k+2}+1\right)+c_{k+1}(1-2^{k+2}+3^{k+1})\;=\;0\,.$$

Therefore,

$$c_{k+1}=(-1)^{k}\frac{\delta^{2k+1}}{(k+1)!}\,,$$

which completes the induction and hence proves (3.5).

Now, we have

$$F(x)\;=\;\sum_{k=1}^{\infty}(-1)^{k+1}\frac{\delta^{2k-1}}{k!}\,x^{k}\;=\;\frac{1}{\delta}\left(1-e^{-\delta^{2}x}\right).$$

Since $\lim_{x\to\infty}F(x)=1$, we obtain $\delta=1$. The proof is complete. □

It is not difficult to see that, conversely, if $X_1\sim\exp(1)$, then (3.1) holds. Indeed, under the assumption of unit exponential parent variable, for the pdf of $X_{3:3}$ we obtain

$$3\,F^{2}(x)\,f(x)\;=\;3\,(1-e^{-x})^{2}\,e^{-x}\;=\;3\bar{F}(x)-6\,\bar{F}(2x)+3\,\bar{F}(3x)\,,$$

which is equivalent to (3.1).

4. SUMS OF DENSITY AND DISTRIBUTION FUNCTIONS

In this section we will prove that (1.3) is a sufficient condition for X_1 to be exponentially distributed. It is straightforward that (1.3) is a necessary condition as well.

Theorem 4.1. *Assume that f is right-continuous at zero. If for $x>0$*

$$\sum_{j=1}^{3}\binom{3}{j}(-1)^{j-1}j\,f(j\,x)\;=\;\sum_{j=1}^{3}\binom{3}{j}(-1)^{j-1}j\,\bar{F}(j\,x)\,, \tag{4.1}$$

then $X_1\sim\exp(1)$.

Proof: The relation (4.1) leads to

$$\big[f(3x)-\bar{F}(3x)\big]-\big[f(2x)-\bar{F}(2x)\big]\;=\;\big[f(2x)-\bar{F}(2x)\big]-\big[f(x)-\bar{F}(x)\big]\,. \tag{4.2}$$

Denoting $Q(y)=f(y)-\bar{F}(y)$, we rewrite (4.2) as

$$Q(y)-Q\Big(\frac{2}{3}\,y\Big)\;=\;Q\Big(\frac{2}{3}\,y\Big)-Q\Big(\frac{1}{3}\,y\Big)\,.$$

Iterating this equation k times and taking limit as $k\to\infty$, we obtain

$$Q(y)-Q\Big(\frac{2}{3}\,y\Big)\;=\;Q\Big(\frac{2}{3}\,y\Big)-Q\Big(\frac{1}{3}\,y\Big)\;=\;\lim_{k\to\infty}Q\bigg(\Big(\frac{2}{3}\Big)^{k}y\bigg)-Q\bigg(\Big(\frac{1}{3}\Big)^{k}y\bigg)\;=\;0\,.$$

This implies $Q(y) = Q(2y/3)$ and thus,

$$Q(y) \;=\; Q\left(\frac{2}{3}\,y\right) \;=\; \lim_{k\to\infty} Q\left(\left(\frac{2}{3}\right)^{k} y\right) \;=\; f(0+) - \bar{F}(0+) \;=\; f(0+) - 1\,. \tag{4.3}$$

On the other hand,

$$\lim_{y\to\infty} f(y) \;=\; \lim_{y\to\infty} f(y) - \lim_{y\to\infty} \bar{F}(y) \;=\; \lim_{y\to\infty} Q(y) \;=\; f(0+) - 1\,. \tag{4.4}$$

But since f is integrable, we have $\lim_{y\to\infty} f(y) = 0$, and therefore, by (4.3) and (4.4), $Q(x) = 0$. Thus, $f(x) = \bar{F}(x)$ for every $x \geq 0$. This, in turn, implies $X_1 \sim \exp(1)$. □

5. SUM AND MAXIMUM OF THREE VARIABLES

It is known (e.g., Arnold *et al.* (2008), p. 77) that if $X \sim \exp\{\lambda\}$, then

$$\sum_{j=1}^{3} \frac{1}{j}\, X_j \overset{d}{=} X_{3:3} \qquad \text{and} \qquad X_{2:2} + \frac{1}{3}\, X_3 \overset{d}{=} X_{3:3}\,. \tag{5.1}$$

We will prove that both relations in (5.1) are also characterization properties of the exponential distribution. Next lemma provides the key argument in the proof of Theorem 1 in [4] and of the theorem below.

Lemma 5.1. *If $F(0) = 0$, the pdf f has a Taylor series expansion for $x > 0$, and*

$$f^{(m)}(0) = \left[\frac{f'(0)}{f(0)}\right]^{m-1} f'(0)\,, \qquad m = 1, 2, \ldots\,, \tag{5.2}$$

then $X_1 \sim \exp\{\lambda\}$ for some $\lambda > 0$.

Proof: For the Taylor series of $f(x)$, using (5.2), we have for $x > 0$

$$f(x) \;=\; \sum_{m=0}^{\infty} \frac{f^{(m)}(0)}{m!}\, x^m \;=\; f(0) + f(0) \sum_{m=1}^{\infty} \left[\frac{f'(0)}{f(0)}\right]^{m} \frac{x^m}{m!} \;=\; f(0) \exp\left\{\frac{f'(0)}{f(0)}\, x\right\}.$$

Since $f(x)$ is a pdf, we have $f'(0)/f(0) < 0$. Denoting $\lambda = -f'(0)/f(0) > 0$ and setting $\int_0^\infty f(x)\, dx = 1$, we obtain $\lambda = f(0)$. Therefore, $f(x) = \lambda e^{-\lambda x}$. □

Next theorem can be obtained as a particular case of the results in [9]. We include it here since it complements the other results for samples of size three given in Theorems 2.1–4.1 and thus provides an easily reference.

Theorem 5.1. *Assume the cdf F admits a power series representation in a neighborhood of zero and $F(0) = 0$.*

(i) *If*

$$X_{2:2} + \frac{1}{3}\, X_3 \overset{d}{=} X_{3:3}\,, \tag{5.3}$$

then $X_1 \sim \exp\{\lambda\}$ for some $\lambda > 0$.

(ii) *If*

$$\sum_{j=1}^{3} \frac{1}{j} X_j \overset{d}{=} X_{3:3}\,, \tag{5.4}$$

then $X_1 \sim \exp\{\lambda\}$ *for some* $\lambda > 0$.

Proof: (i). The pdf of the left-hand side of (5.3) is

$$\begin{aligned} f_{X_{2:2}+X_3/3}(x) &= \int_0^x f_{X_3/3}(y)\, f_{X_{2:2}}(x-y)\, dy \\ &= \int_0^x 3\, f(3y)\, \frac{d}{dx}\left[F^2(x-y)\right] dy \\ &= 6 \int_0^x f(3y)\, F(x-y)\, f(x-y)\, dy\,. \end{aligned} \tag{5.5}$$

For the pdf of the right-hand side of (5.3), we have

$$f_{X_{3:3}}(x) \;=\; 3\, F^2(x)\, f(x) \;=\; 6\, f(x) \int_0^x F(y)\, f(y)\, dy\,. \tag{5.6}$$

Let $G(x) := F(x)\, f(x)$. It follows from (5.5) and (5.6) that (5.3) is equivalent to

$$\int_0^x f(3y)\, G(x-y)\, dy \;=\; f(x) \int_0^x G(y)\, dy\,. \tag{5.7}$$

Differentiating the left-hand side of (5.7) n times with respect to x, we obtain

$$\frac{d^n}{dx^n} \int_0^x f(3y)\, G(x-y)\, dy \;=\; \sum_{i=1}^{n} f^{(n-i)}(3x)\, G^{(i-1)}(0) + \int_0^x f(3y)\, G^{(n)}(x-y)\, dy\,.$$

Applying the Leibniz rule for the n-th derivative of a product of two functions to the right-hand side of (5.7), we obtain

$$\frac{d^n}{dx^n} \left[f(x) \int_0^x G(y)\, dy \right] \;=\; \sum_{i=1}^{n} \binom{n}{i} f^{(n-i)}(x)\, G^{(i-1)}(x) \;+\; f^{(n)}(x) \int_0^x G(y)\, dy\,.$$

In the last two equations letting $x = 0$, we have

$$\sum_{i=1}^{n} 3^{n-i} f^{(n-i)}(0)\, G^{(i-1)}(0) \;=\; \sum_{i=1}^{n} \binom{n}{i} f^{(n-i)}(0)\, G^{(i-1)}(0)\,. \tag{5.8}$$

Since $G(0) = 0$ and $G'(0) = f^2(0)$, the above equation is equivalent to

$$\left[3^{n-2} - \binom{n}{2}\right] f^{(n-2)}(0)\, f^2(0) \;=\; \sum_{i=3}^{n} \left[\binom{n}{i} - 3^{n-i}\right] f^{(n-i)}(0)\, G^{(i-1)}(0)\,, \tag{5.9}$$

where $n \geq 4$. We will prove that (5.9) implies (5.2). Equation (5.2) is trivially true for $m = 1$. To proceed by induction, assume (5.2) holds true for all $1 \leq m \leq n-3$, where $n \geq 4$. We need to prove it for $m = n-2$. Using the induction assumption, it is not difficult to obtain for $j = 1, 2, ..., n-2$

$$G^{(j)}(0) \;=\; \sum_{i=0}^{j} \binom{j}{i} F^{(i)}(0)\, f^{(j-i)}(0) \;=\; f^2(0) \left[\frac{f'(0)}{f(0)}\right]^{j-1} (2^j - 1)\,.$$

Therefore, using the induction assumption again, we have for $i = 3, 4, ..., n-1$

$$f^{(n-i)}(0)\,G^{(i-1)}(0) \;=\; \left[\frac{f'(0)}{f(0)}\right]^{n-3} f'(0)\,f^2(0)\,(2^{i-1}-1)\,. \tag{5.10}$$

Substituting this in the right-hand side of (5.9) yields

$$\left[3^{n-2} - \binom{n}{2}\right] f^{(n-2)}(0) \;=\; \left[\frac{f'(0)}{f(0)}\right]^{n-3} f'(0) \sum_{i=3}^{n} \left[\binom{n}{i} - 3^{n-i}\right](2^{i-1}-1)\,.$$

To complete the proof of (5.2), it is sufficient to show that

$$3^{n-2} - \binom{n}{2} \;=\; \sum_{i=3}^{n} \left[\binom{n}{i} - 3^{n-i}\right](2^{i-1}-1)\,,$$

which can be easily verified. This proves (5.2). The claim in (i) follows from (5.2) and the lemma. □

Proof: (**ii**). Equation (5.4) is equivalent to

$$6\int_0^z f(y)\int_0^{z-y} f(2x)\,f\big(3(z-y-x)\big)\,dx\,dy \;=\; 6\,f(z)\int_0^z F(y)\,f(y)\,dy\,. \tag{5.11}$$

Denoting

$$H(z-y) \;:=\; \int_0^{z-y} f(2x)\,f\big(3(z-y-x)\big)\,dx\,, \tag{5.12}$$

we write (5.11) as

$$\int_0^z f(y)\,H(z-y)\,dy \;=\; f(z)\int_0^z G(y)\,dy\,. \tag{5.13}$$

Similarly to the proof of (i), differentiating n times both sides of (5.13) with respect to z and setting $z = 0$, we have

$$\sum_{i=1}^{n-1} f^{(n-1-i)}(0)\,H^{(i)}(0) \;=\; \sum_{i=1}^{n-1}\binom{n}{i+1} f^{(n-1-i)}(0)\,G^{(i)}(0)\,.$$

Since $H'(0) = G'(0) = f^2(0)$, the last equation can be written for $k = n-1$ as

$$\left[1 - \binom{k+1}{2}\right] f^{(k-1)}(0)\,f^2(0) \;=\; \sum_{i=2}^{k}\left[\binom{k+1}{i+1} G^{(i)}(0) - H^{(i)}(0)\right] f^{(k-i)}(0)\,. \tag{5.14}$$

Now we are in a position to prove (5.2) by induction. (5.2) holds true for $m = 1, 2, ..., k-2$. Differentiating (5.12) with respect to z and setting $z = y$, we have

$$H^{(n)}(0) \;=\; \sum_{i=1}^{n} 2^{n-i} f^{(n-i)}(0)\;3^{i-1} f^{(i-1)}(0)\,. \tag{5.15}$$

Under the induction assumption, (5.15) implies for $j = 1, 2, ..., n-2$

$$H^{(j)}(0) = \left[\frac{f'(0)}{f(0)}\right]^{j-1} f^2(0)\,(3^j - 2^j)\,.$$

Using the induction assumption again, we have for $i = 3, 4, ..., n-1$

$$f^{(n-i)}(0)\,H^{(i-1)}(0) \;=\; \left[\frac{f'(0)}{f(0)}\right]^{n-3} f'(0)\,f^2(0)\,(3^{i-1} - 2^{i-1})\,.$$

Recalling (5.10) from the proof of (i), we rewrite (5.14) as (note that $i = n$ corresponds to a 0 term)

$$\left[1 - \binom{n}{2}\right] f^{(n-2)}(0) \;=\; \left[\frac{f'(0)}{f(0)}\right]^{n-3} f'(0) \sum_{i=3}^{n} \left[\binom{n}{i}(2^{i-1} - 1) - (3^{i-1} - 2^{i-1})\right].$$

Thus, to prove (5.2) for $k = n-2$ it is sufficient to show that

$$1 - \binom{n}{2} \;=\; \sum_{i=3}^{n} \left[\binom{n}{i}(2^{i-1} - 1) - (3^{i-1} - 2^{i-1})\right],$$

which verifies. This proves (5.2), which referring to the lemma, completes the proof of (ii). □

6. EXAMPLE

We will illustrate a possible application of Theorem 5.1 with an example (see also [4]). Assume we have a simple random sample $X_1, X_2, ..., X_n$ for $n \geq 6$. Let us randomly divide the data set into six subsets, relabeled as

$$U_1, U_2, ..., U_{n/6}\,, \qquad V_1, V_2, ..., V_{n/6}\,, \qquad W_1, W_2, ..., W_{n/6}\,,$$
$$X_1, X_2, ..., X_{n/6}\,, \qquad Y_1, Y_2, ..., Y_{n/6}\,, \qquad Z_1, Z_2, ..., Z_{n/6}\,.$$

Define for $i = 1, 2, ..., n/4$

$$R_i := U_i + \frac{1}{2}V_i + \frac{1}{3}W_i\,, \qquad S_i := \max\{U_i, V_i\} + \frac{1}{3}W_i \quad \text{and} \quad T_i := \max\{X_i, Y_i, Z_i\}\,.$$

Then, according to Theorem 5.1, the R's, the S's, and the T's will have a common distribution if and only if the original X's follow an exponential distribution.

Let us simulate a sample of size $n = 180$ from a parent variable with exp(1) distribution. The values of R_i, S_i, and T_i for $i = 1, 2, ..., 30$ are presented in Table 1.

Using the non-parametric two-sample Wicoxon rank test, we compare the sample distribution functions of the R's and T's on one hand and the S's and T's on another. The test results provide evidence supporting an exponential underlying distribution. Namely, the hypothesis that the distributions of the R's and the T's are the same cannot be rejected with p-value 0.7635 ($W = 471$). The hypothesis that the distributions of the S's and the T's are the same cannot be rejected with p-value 0.9357 ($W = 444$).

Table 1: Values R_i, S_i, and T_i for $i = 1, 2, ..., 30$.

R	3.56	0.70	0.62	3.33	0.30	0.78	2.29	0.97	1.59	0.50
	0.83	2.27	0.69	2.95	0.32	4.12	0.74	0.91	2.66	0.48
	2.87	2.19	2.32	1.08	3.69	1.98	1.13	1.32	3.37	2.73
S	2.98	1.23	0.77	2.75	0.44	0.75	1.97	1.08	1.43	0.50
	0.76	1.65	0.58	2.39	0.27	3.41	0.73	0.89	2.63	0.40
	2.22	1.87	4.25	1.07	2.72	1.74	1.07	1.11	2.71	3.87
T	2.07	0.60	0.97	0.47	2.84	0.84	1.02	1.84	0.57	2.88
	1.39	1.92	8.46	1.77	2.60	1.42	1.50	0.47	0.26	2.17
	1.92	1.67	2.87	1.06	2.24	6.63	0.52	1.09	1.33	1.07

7. CONCLUDING REMARKS

In this paper we proved characterizations of the exponential distribution conjectured by Arnold and Villaseñor in [4]. Furthermore, under the assumptions of Theorem 2.1 and using the same technique of proof, it can be seen that if $X_1 + \frac{1}{2}X_2 + \frac{1}{3}X_3$ has as its density any one of the following seven forms, then X_i's are exponential:

$$\begin{aligned}
&3\,f(x) - 6\,f(2x) + 3\,\bar{F}(3x)\,, &&3\,f(x) - 6\,\bar{F}(2x) + 3\,f(3x)\,,\\
&3\,\bar{F}(x) - 6\,f(2x) + 3\,f(3x)\,, &&3\,f(x) - 6\,\bar{F}(2x) + 3\,\bar{F}(3x)\,,\\
&3\,F(x) - 6\,f(2x) + 3\,\bar{F}(3x)\,, &&3\,\bar{F}(x) - 6\,\bar{F}(2x) + 3\,f(3x)\,,\\
&3\,\bar{F}(x) - 6\,\bar{F}(2x) + 3\,\bar{F}(3x)\,.
\end{aligned}$$

Likewise, under the assumptions of Theorem 3.1 and using the same technique of proof, it can be obtained that if $X_{3:3}$ has as its density any one of the preceding seven forms, then X_i's are exponential.

The results presented here can be extended in several directions. Naturally, one would like to explore the general case of samples of size n for any $n \geq 4$. As we mentioned earlier, generalizations of Theorem 5.1 for arbitrary sample size are proved in [9]. Here we would like to propose as open problems the following two characterizations, which would extend Theorem 2.1 and Theorem 3.1, respectively.

Proposition 7.1. *Let $X_1, X_2, ..., X_n$ be i.i.d. random variables, where $n \geq 4$. Assume $\varphi(t)$ is finite for all t in a neighbourhood of zero. If for $x > 0$*

$$\sum_{j=1}^{n} \frac{1}{j} X_j \quad \textit{has pdf} \quad \sum_{j=1}^{n} \binom{n}{j} (-1)^{j-1} j\, f(j\,x)\,,$$

then $X_1 \sim \exp(\lambda)$ for some $\lambda > 0$.

Proposition 7.2. *Let $X_1, X_2, ..., X_n$ be i.i.d. random variables, where $n \geq 4$. Assume the cdf F has a power series representation in a neighborhood of zero. If for $x > 0$*

$$X_{n:n} \quad \text{has pdf} \quad \sum_{j=1}^{n} \binom{n}{j} (-1)^{j-1} j \, \bar{F}(j\,x)\,,$$

then $X_1 \sim \exp(1)$.

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TESTING FOR TRENDS IN EXCESSES OVER A THRESHOLD USING THE GENERALIZED PARETO DISTRIBUTION

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Abstract:

- The Generalized Pareto Distribution (GPD) is used for modeling exceedances over thresholds. The general form of the GPD depends on three parameters: the location parameter μ; the scale parameter ($\beta > 0$); and the shape parameter ($-\infty < \xi < \infty$). This work restricts attention to the case where $\mu = 0$ and shows that, as ξ decreases while β is kept fixed, the family of GPD(ξ, β) distributions increases in the usual stochastic order. This property is used for testing the significance of trends in the size of the exceedances over high thresholds in a time series consisting of ozone measurements.

Key-Words:

- *Stochastic Order; Peaks Over a Threshold; Ozone Concentrations; Likelihood Ratio Tests.*

1. INTRODUCTION

Let X be a random variable with continuous distribution function F and corresponding survival function $\bar{F} = 1 - F$. Let x^* be the right endpoint of the support of F defined by $x^* = \sup\{x \in \mathbb{R} \colon F(x) < 1\}$. Given a real number $u < x^*$, referred to as the threshold, an *exceedance* over the threshold u occurs when $X > u$. The residual life function of F at time u, the probability that $X > u + x$ given that $X > u$, is

$$(1.1) \qquad \bar{F}_u(x) = P\big(X - u > x \mid X > u\big) = \frac{\bar{F}(x+u)}{\bar{F}(u)}, \qquad 0 < x < x^* - u .$$

The random variable $X - u$ is called the *excess* over the threshold u and $\bar{F}_u$ is the *excess* survival function of X over u. When F belongs to the domain of attraction of one of the extreme value distributions, it follows that, for sufficiently large u, the distribution function of $X - u$ can be approximated by the Generalized Pareto Distribution (GPD). The distribution function of a GPD(ξ, β) is

$$(1.2) \qquad F(x;\xi,\beta) = \begin{cases} 1 - (1 - \xi x/\beta)^{1/\xi}, & \xi \neq 0\,, \ \beta > 0\,, \\[2ex] 1 - \exp(-x/\beta)\,, & \xi = 0\,, \ \beta > 0\,, \end{cases}$$

where ξ and β are the shape and scale parameters, respectively. When $\xi < 0$ the support of $F(x;\xi,\beta)$ consists of the positive reals. When $\xi > 0$, the support is the interval $(0, \beta/\xi)$. The case $\xi = 0$ corresponds to the exponential distribution with mean β. When $\xi = 1$, the GPD distribution corresponds to the uniform distribution on $[0, \beta]$.

More precisely, let $X_1, ..., X_n$ be a sequence of independent and identically distributed random variables with continuos distribution H. Let $M_n = \max\{X_1, ..., X_n\}$. Suppose that there are sequences $a_n > 0$ and b_n of real numbers such that

$$(1.3) \qquad P\big\{a_n(M_n - b_n) \leq z\big\} \to G(z)\,, \qquad \text{as} \quad n \to \infty\,.$$

Then $G(z)$ is a member of the generalized extreme value distribution family defined by

$$G(z) = \exp\left\{-\left\{1 - \xi\left(\frac{z-\mu}{\sigma}\right)\right\}^{1/\xi}\right\}.$$

The precise technical justification for modeling excesses using the GPD — expression (1.2) — was provided by Smith [32] and is based on the fact that

$$\lim_{u \to x^*} \sup_{0<x<x^*-u} \big|F_u(x) - F\big(x;\xi,\beta(u)\big)\big| = 0\,,$$

for fixed ξ and some positive function $\beta(u)$, if and only if F is in the domain of attraction of some extreme value distribution. This result is from the parallel work done by Balkema and de Haan [1] and Pickands [23]. Since most of the common continuous distributions belong to the domain of attraction of one of the three extreme value distributions, this result makes the GPD the natural model for the excess distribution of the random variable X when the threshold is high.

Starting with the early works by Smith [31] and Davison [6], the GPD has been used by many authors to model excesses over high thresholds in several fields such as river floods, air pollution, wind velocity, sea waves, insurance claims, etc. For the details of these applications see Hosking and Wallis [12], Smith [33], Dargahi-Noubary [5], Grimshaw [10], Rootzen and Tajvidi [29], Castillo and Hady [4], and Parisi and Lund [22]. Embrechts *et al.* [8], Falk *et al.* [9], and Reiss and Thomas [24] present detailed and elegant accounts of the theoretical underpinnings and the practical aspects of the modeling of extremes including discussions on the modeling of exceedances and excesses.

One of the main objectives of modeling excesses over high thresholds with the GPD is the estimation of tails of probability distributions — Smith [32]. But the GPD has also been used to detect and test for trends in the excesses. The papers by Smith [33], Davison and Smith [7], Smith and Huang [35] and Rootzen and Tajvidi [29] are some examples of such applications. Our interest in this article is also in testing for the existence of a long term trend in the excesses of a time series. The main difference with other works is our use of the concept of stochastic orderings of distribution functions. In Section 2 it is shown that given k GPD distributions $F(\cdot;\xi_j,\beta)$, $(j=1,...,k)$, if $\xi_1<\xi_2<\cdots<\xi_k$, then $F(x;\xi_1,\beta)>F(x;\xi_2,\beta)>\cdots>F(x;\xi_k,\beta)$ for all x. That is, we give a sufficient condition for the GPD family to be stochastically ordered. This condition is used in Section 3 to develop a simple procedure based on a likelihood ratio statistic for testing $H_0\colon\ \xi_1=\xi_2=\cdots=\xi_k$ *vs.* the isotonic alternative $H_a\colon\ \xi_1\le\xi_2\le\cdots\le\xi_k$. Our procedure is desirable when it is believed a priori that the GPDs satisfy the stochastic order restriction and, hence, it is desirable to have a test that is more powerful than an omnibus test.

The test being proposed here belongs to the field of restricted inference. There is a vast literature in this area. The literature consists of roughly two large subareas: shaped-restricted inference, and order-restricted inference. Barlow *et al.* [2] is a classic pioneering work based on isotonic regression ideas and the Pool-Adjacent-Violators-Algorithm. Robertson *et al.* [25] and the many references therein, summarize and extend the work of Barlow *et al.* and adopt the Nonparametric Maximum Likelihood paradigm proposed by Kiefer and Wolfowitz [14]. Kiefer and Wolfowitz [15] seem to have pioneered the area of shape-restricted inference. Wang [36, 37, 38], extended ideas of Kiefer and Wolfowitz to the estimation of distribution functions under the restriction of being star-shaped or being Increasing Failure Rate on Average. Lo [19], Rojo [26, 27], and Rojo and Ma [28], provide nonparametric estimators for distribution functions that are stochastically ordered. One recent monograph that examines shape-restricted inference is Groeneboom and Jongbloed [11]. Marshall and Olkin [20] and Shaked and Shanthikumar [30] provide excellent treatises on the topic of partial orders of distribution functions.

Finally, in Section 4, we apply our procedure to test for the existence of a monotonic trend in the size of the excesses of a time series of ozone measurements.

2. STOCHASTIC ORDERING OF THE GPD

The concept of stochastic order permeates the theory and applications of statistics. The concept was introduced in the seminal paper by Lehmann [17] and was used to study the power properties of certain tests.

Definition 2.1. Let X and Y be random variables such that

$$P(X > x) \leq P(Y > x)\,, \qquad -\infty < x < \infty\,.$$

Then X is said to be *stochastically smaller* than Y. This is denoted by $X <^{\mathrm{st}} Y$.

We can also state that Y is stochastically larger than X and write $Y >^{\mathrm{st}} X$. If F and G represent the cumulative distribution functions (*cdfs*) of X and Y respectively, then $X <^{\mathrm{st}} Y$ if and only of $F(x) \geq G(x)$ for all $x \in \mathbb{R}$, and then we write $F <^{\mathrm{st}} G$. As discussed by Lehmann [17], a convenient situation arises when the stochastic order is induced by the parameter as it varies monotonically in the parameter space. That is, a parametric family of cdfs $\{F(x;\theta) : \theta \in \Theta \subset \mathbb{R}\}$ is stochastically increasing in θ if $\theta_1 < \theta_2$ implies that $F(\cdot;\theta_1) <^{\mathrm{st}} F(\cdot;\theta_2)$. Similarly, $\{F(x;\theta) : \theta \in \Theta \subset \mathbb{R}\}$ is stochastically decreasing in θ if $\theta_1 < \theta_2$ implies that $F(\cdot;\theta_2) <^{\mathrm{st}} F(\cdot;\theta_1)$. Lehmann and Rojo [18] provided simple characterizations of this and other related orders.

Sufficient conditions are provided here for the family of GPD distribution functions $\mathcal{F} = \{F(x;\xi,\beta) : -\infty < \xi < \infty,\ \ \beta > 0\}$, to be stochastically ordered. Since β is a scale parameter it is clear that the family $\mathcal{F}$ is stochastically ordered in β for fixed ξ. The following Proposition states that the family $\mathcal{F}$ is stochastically decreasing in ξ for fixed β.

Proposition 2.1. *Let $F_1, F_2 \in \mathcal{F}$ with shape parameters ξ_1 and ξ_2, respectively and equal scale β. If $\xi_1 < \xi_2$ then $F_2 <^{\mathrm{st}} F_1$.*

Proof: The proof of Proposition 2.1 uses the following result.

Proposition 2.2 (Mitrinovic [21], pp. 266, inequality 3.6.1)**.** *If $a > 0$ and $x > 0$, then*

$$e^{-x} \leq \left(\frac{a}{ex}\right)^{a}. \tag{2.1}$$

Setting $x = 1/u$ and $a = 1$ in (2.1) we obtain

$$u \geq e^{1-1/u}\,, \qquad u > 0\,. \tag{2.2}$$

Now we prove Proposition 2.1. Let $F(\cdot;\xi,\beta) \in \mathcal{F}$ for β fixed. From the definition of the usual stochastic order, it is enough to show that $F(\cdot;\xi,\beta)$ is an increasing function of the parameter $\xi \in \mathbb{R}$. This is true if and only if

$$h(\xi) \;=\; \log\bigl[1 - F(x;\xi,\beta)\bigr] \;=\; (1/\xi)\log(1 - \xi x/\beta)$$

is a decreasing function. First we analyze the case $\xi \neq 0$, for which the problem reduces to showing that

$$h'(\xi) \;=\; -(1/\xi^2)\log(1 - \xi x/\beta) - \frac{x}{\xi\beta(1 - \xi x/\beta)} \;<\; 0\,. \tag{2.3}$$

Making the change of variable $u = 1 - \xi x/\beta$ we get $h'(\xi) = h'\bigl(\beta(1-u)/x\bigr) = g(u)$, where

$$g(u) \;=\; -\bigl[x/\beta(1-u)\bigr]^2 \bigl(\log u + (1/u) - 1\bigr)\,,$$

for $0 < u < 1$ when $\xi > 0$, and $1 < u < \infty$ when $\xi < 0$. Then, $g(u) < 0$ if and only if $\log u + (1/u) - 1 > 0$, if and only if $u > e^{1-1/u}$, $u > 0$. But this is the strict inequality in (2.2). Hence (2.3) holds and therefore $F(x;\xi,\beta)$ is increasing in ξ for $\xi \in \mathbb{R}\backslash\{0\}$. Now

$$\lim_{\xi\to 0}\Big\{1-(1-\xi x/\beta)^{1/\xi}\Big\} = 11 - e^{-x/\beta} .$$

This means that $F(x;\xi,\beta) \uparrow F(x;\xi\!=\!0,\beta)$ as $\xi \uparrow 0$, and $F(x;\xi,\beta) \downarrow F(x;\xi\!=\!0,\beta)$ as $\xi \downarrow 0$. Then, from the proved monotonicity of $F(x;\xi,\beta)$ in $\xi \in \mathbb{R}\backslash\{0\}$, the proposition follows. □

Thus, the following result is obtained.

Corollary 2.1. *Let $F(x;\xi;\beta)$ denote the GPD distribution with scale parameter β and shape parameter ξ as defined by (1.2). Then,*

If $\xi^* = \xi$ and $\beta < \beta^*$, $F(\cdot;\xi^*,\beta^*) \geq^{\rm st} F(\cdot;\xi,\beta)$.

If $\xi > \xi^*$ and $\beta = \beta^*$, $F(\cdot;\xi^*,\beta^*) \geq^{\rm st} F(\cdot;\xi,\beta)$.

When $\xi > -1$, the expected value μ of a $\mathrm{GPD}(\xi,\beta)$ is $\mu = \beta(1+\xi)^{-1}$. Then $\xi = \xi(\mu) = (\beta/\mu) - 1$. Thus the shape parameter ξ is a decreasing function of the mean μ. So, if $X_1 \sim \mathrm{GPD}(\xi_1,\beta)$ and $X_2 \sim \mathrm{GPD}(\xi_2,\beta)$, with $\xi_1, \xi_2 > -1$, and we assume that the means $\mu_j = EX_j$ $(j = 1,2)$ are such that $\mu_2 \leq \mu_1$, then $\xi_1 < \xi_2$. Thus if $\mu_2 \leq \mu_1$ then $X_2 <^{\rm st} X_1$. The converse is also true. To see this, let F_j be the cdf of X_j and assume $X_2 <^{\rm st} X_1$, then we have $1 - F_2(x) \leq 1 - F_1(x)$ for all x, and since the GPD only takes positive values, it follows that

$$\mu_2 \;=\; \int_0^\infty \big[1 - F_2(x)\big]\, dx \;\leq\; \int_0^\infty \big[1 - F_1(x)\big]\, dx \;=\; \mu_1 \,.$$

We can put together all these results in the following corollary.

Corollary 2.2. *Let $X_j \sim GPD(\xi_j,\beta)$, (or if $X_j \sim GPD(\xi,\beta_j)$), $(j = 1,...,k)$. Suppose that $E(X_j) = \mu_j$ exists for all j. Then the following propositions are equivalent.*

a) $X_1 \overset{\rm st}{>} X_2 \overset{\rm st}{>} \cdots \overset{\rm st}{>} X_k$.

b) $\xi_1 < \xi_2 < \cdots < \xi_k$, $(\beta_1 > \beta_2 > \cdots > \beta_k)$.

c) $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_k$.

3. TESTING FOR A LINEAR TREND IN THE EXCESSES

Let $X_j \sim \mathrm{GPD}(\xi_j,\beta)$, $(j = 1,...,k)$, and denote equality in distribution by $\overset{\mathcal{D}}{=}$. Suppose we want to test the null hypothesis

$$H_0\colon\; X_1 \overset{\mathcal{D}}{=} X_2 \overset{\mathcal{D}}{=} \cdots \overset{\mathcal{D}}{=} X_k$$

vs. the alternative

$$H_a\colon\; X_1 >^{\rm st} X_2 >^{\rm st} \cdots >^{\rm st} X_k \,.$$

From Corollary 2.2, we see that this would be equivalent to testing the null hypothesis

$$H_0\colon \;\; \xi_1 = \xi_2 = \cdots = \xi_k$$

vs. the alternative hypothesis

$$H_a\colon \;\; \xi_1 < \xi_2 < \cdots < \xi_k \,.$$

Similarly, the hypothesis $H_a\colon X_1 <^{\text{st}} X_2 <^{\text{st}} \cdots <^{\text{st}} X_k$ can be tested by using $H_a\colon \xi_1 > \xi_2 > \cdots > \xi_k$. From Corollary 2.2, a test for the stochastic order could also be based on the means of the GPD's. However the means do not always exist. Therefore we test the hypothesis of stochastic order on the basis of the shape parameter. Assume that for each X_j we have a random sample of size n_j, $x_j = (x_{1j}, ..., x_{n_j j})'$ and let $x = (x_1, x_2, ..., x_k)$ be the full data vector. Furthermore, assume that we observe the X_j's sequentially along time, and let t_j be the epoch at which the random sample x_j was observed. To detect a linear time trend, we introduce a third parameter θ by writing $\xi_j = \xi + \theta t_j$, $(j = 1, ..., k)$. When the t_j's are equally spaced, t_j can be set as $t_j = j$. Thus, we can test the hypothesis of order restriction by testing

$$H_0\colon \;\; \theta = 0$$

vs. the alternative hypothesis

$$H_a\colon \;\; \theta \neq 0 \,. \tag{3.1}$$

Although other forms of monotonic trends could occur, e.g. $\xi_j = \xi \exp(\theta t_j)$, a test without assuming a particular form of the monotone trend would require a semiparametric model that would provide protection against misspecification of the functional form of the trend but would not perform as well as the current test for the specific alternative of a monotonic linear trend.

Modeling the parameters of the GPD in order to assess a trend is similar to the approach described in other works such as those by Smith [34], Smith and Huang [35] and Rootzen and Tajvidi [29]. For instance, Rootzen and Tajvidi model the scale parameter as $\beta = \exp(\alpha_0 + \alpha_1 t)$ where t is time in years, and keep the shape parameter ξ constant. In this work we reverse this procedure.

Let $\underset{\sim}{X}$ represent the data vector $X_1, X_2, ..., X_n$. For testing the hypothesis (3.1), we use the Likelihood Ratio Test (LRT) based on $\lambda(\underset{\sim}{X}) = L(\hat{\xi}, \hat{\beta})/L(\hat{\xi}, \hat{\theta}, \hat{\beta})$, where L denotes the likelihood function and the estimators are maximum likelihood estimators (MLE). Then $-2 \log \lambda(\underset{\sim}{X})$ follows asymptotically a chi-square distribution with one degree of freedom. The detailed expression for $-2 \log \lambda(\underset{\sim}{X})$ is given in the Appendix.

4. AN APPLICATION TO OZONE DATA

The data we analyze was collected in Yosemite National Park Wanona Valley and consists of hourly measurements of ozone (ppm) taken from April 1, 1987 to October 31, 1996. The time series contains 84,011 observations with 9412 missing values. The main concern is the detection of a long term trend in the extremal behavior of the time series.

More precisely, the problem is to detect either a decreasing or increasing trend in the size of the excesses over a certain high threshold, if in fact a trend exists. Table 1 displays the monthly number of exceedances over 0.08 ppm. The observations have a strong seasonal component with two periods: the exceedances period which extends from the month of April trough the month of October and the no-exceedances period in the remaining months. The frequency of exceedances increases in the summer months and then decreases in the fall months. Moreover, exploring the data we found that the ozone levels also tend to increase in the summer months and decrease in the fall months. Since the interest lies on the extremal behavior of the data, the analysis was based on the months from April to October.

Table 1: Monthly exceedances over 8 ppm.

Year	Apr	May	Jun	Jul	Aug	Sep	Oct	Total (N_u)	n
1987	4	14	70	55	75	50	23	291	4742
1988	9	2	11	83	71	92	21	289	4856
1989	0	6	9	32	29	7	0	83	4913
1990	1	8	34	91	65	63	3	265	4630
1991	0	0	2	19	1	38	17	77	4463
1992	0	2	14	27	49	21	11	124	4736
1993	0	0	3	20	11	21	0	55	3860
1994	6	6	3	14	3	0	0	32	4720
1995	0	0	0	6	50	27	0	83	4804
1996	0	0	4	39	29	22	2	96	4636
Total	20	38	150	386	383	341	77	1395	46360

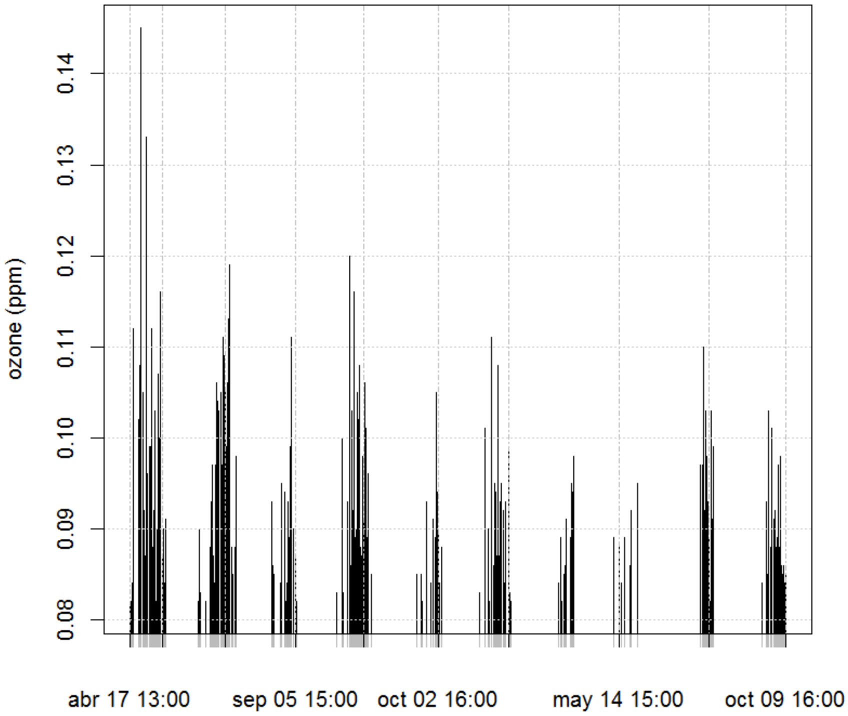

Figure 1: Excesses over 0.08 ppm.

Figure 1 shows the empirical marked point processes of exceedances over 0.08 ppm. A clear decreasing trend in the size of the excesses appears. We assess the significance of this trend using the LRT from Section 3.

The LRT requires the excesses to be independent of one another. There is, however, a strong dependence between the exceedances because they tend to occur in clusters. That is, an exceedance tends to attract other exceedances. Several procedures to deal with dependent data have been proposed. One such procedure is to identify clusters of exceedances for which it can be assumed that the excesses within any cluster are independent of the excesses within any other cluster, and then select the maximum excesses within each cluster.

The practical problem with this approach is the identification of independent clusters. Two methods have been used. One is to select a time length b (called block length) and then partition all the observations into consecutive blocks of length b. Then consider all the exceedances within a block as a cluster of exceedances. These are called block-clusters. See Leadbetter [16] for the formal justification of this approach as well as for some applications.

The second approach is to select a positive integer r (called the run length) and then decide that any run of at least r consecutive observations below the threshold separates two clusters of exceedances and then assume that such clusters are independent. These are called run-clusters. See Smith [33] for an application of this approach. In this work we use the run-cluster approach with 72 hours (three days) separation. This window of 72 hours is the common practice when analyzing ozone data. Once we have identified the run clusters, we take the maximum excess within each cluster. To distinguish from the *Exceedances over a Threshold* we call these values the *Peaks over a Threshold*, (POT's). Table 2 shows the POT's that we analyze in this work.

Table 2: POT, run-clusters, 72 hours.

Year	Peaks									
1987	0.002	0.004	0.032	0.022	0.065	0.025	0.053	0.032	0.027	0.036
	0.010	0.011								
1988	0.002	0.010	0.002	0.013	0.017	0.007	0.017	0.026	0.023	0.025
	0.031	0.039	0.008	0.018						
1989	0.013	0.005	0.015	0.014	0.004	0.013	0.009	0.019	0.031	0.010
	0.007	0.002								
1990	0.003	0.020	0.003	0.013	0.040	0.036	0.007	0.018	0.026	0.016
	0.005									
1991	0.005	0.005	0.002	0.013	0.004	0.011	0.007	0.025	0.010	0.008
1992	0.003	0.021	0.010	0.031	0.006	0.015	0.007	0.028	0.012	0.013
	0.019	0.003	0.002							
1993	0.004	0.009	0.011	0.009	0.015	0.018				
1994	0.009	0.008	0.004	0.009	0.006	0.012	0.015			
1995	0.017	0.017	0.030	0.023	0.018	0.009	0.023	0.011	0.019	
1996	0.004	0.013	0.023	0.021	0.012	0.009	0.017	0.018	0.006	0.006
	0.004	0.005								

Figure 2 shows the POT's for all the years of the observation period. The decreasing trend in the POT's is evident. Under H_0 the estimates of the parameters are $\hat{\xi} = 0.2121$ and

$\hat{\beta} = 0.0179$. Under H_a we have $\hat{\xi} = 0.164$, $\hat{\theta} = 0.0575$, and $\hat{\beta} = 0.0209$. The positive value of the estimate of ξ is consistent with the observed decrease in the excesses of the ozone levels. The observed value of the LRT is $-2\log\lambda(x) = 17.24$ which has a p-value of 0.000033. Thus we conclude that the observed decrease in the size of the excesses from 1987 to 1996 is statistically significant.

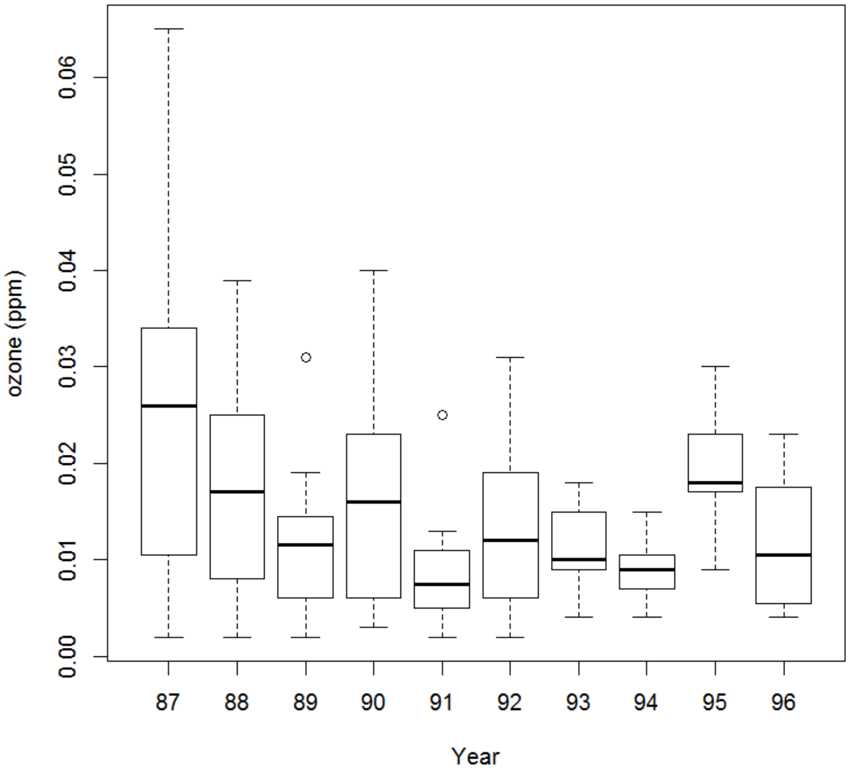

Figure 2: Maximum excesses within run-clusters grouped by years.

Once we have found statistical evidence for the decreasing trend in the excesses, we estimate the upper tail of the ozone levels as in Davison and Smith [7] or Embrechts *et al.* [8]. From (1.1) one gets

$$1 - F(u+x) = \gamma_u\big[1 - F_u(x)\big]\,,$$

where $\gamma_u = \Pr(X > u) = 1 - F(u)$. Thus, if N_u is the number of exceedances over u and n is the number of observations, then an estimator of γ_u is $\hat{\gamma}_u = N_u/n$, and an estimator of the upper tail of F_X is given by

$$(4.1) \qquad 1 - \hat{F}(u+x) = \hat{\gamma}_u\big[1 - \hat{F}_u(x)\big] = \frac{N_u}{n}\left(1 - \hat{\xi}\,\frac{x}{\hat{\beta}}\right)^{1/\hat{\xi}}, \qquad x > 0\,.$$

Estimators of the quantiles of F are obtained by solving $\hat{F}(x_p) = p$ for x_p in (4.1), $0 \le p \le 1$. This yields

$$(4.2) \qquad \hat{x}_p = u + \frac{\hat{\beta}}{\hat{\xi}}\left[1 - \left(\frac{n(1-p)}{N_u}\right)^{\hat{\xi}}\,\right].$$

When $\hat{\xi} > 0$ by setting $p = 1$ we obtain the estimator of the right end point $\hat{x}^* = u + \hat{\beta}/\hat{\xi}$.

The ozone levels are not independent. So, to simplify, we assume that within the exceedances period in the year (from April to October) the ozone levels come from a strongly stationary process. Then, from the Ergodic Theorem — see Breiman [3], pp. 118 —, we have that $(1/n)\sum_{i=1}^{n} 1_{\{X_i>u\}} = N_u/n$ converges almost surely to $1-F(u)$, where now F is the marginal distribution of the ozone levels. Thus N_u/n may be used as an estimator of $1-F(u)$, and then we can use (4.2) to estimate the upper tail and high quantiles of the distribution of the ozone levels. Table 3 shows the estimates of the shape parameters and from Table 1 we get the number of observations (ozone measurements) and the number of exceedances per year. With this information we can estimate the extreme quantiles of the ozone levels. For instance, for 1987, we have

$$\hat{x}_p = 0.08 + (0.0209)\Big(1 - \big[4742\,(1-p)/291\big]^{0.22}\Big)/0.22\,, \qquad 0 \le p \le 1\,.$$

Figure 3 shows the estimated 0.99, 0.999 quantiles as well as the right endpoints of the marginal distribution of the ozone levels. The decreasing trend is evident.

Table 3: Estimated shape parameters.

t_j	1	2	3	4	5	6	7	8	9	10
$\hat{\xi}_j$	.22	.278	.336	.394	.452	.51	.568	.626	.684	.742

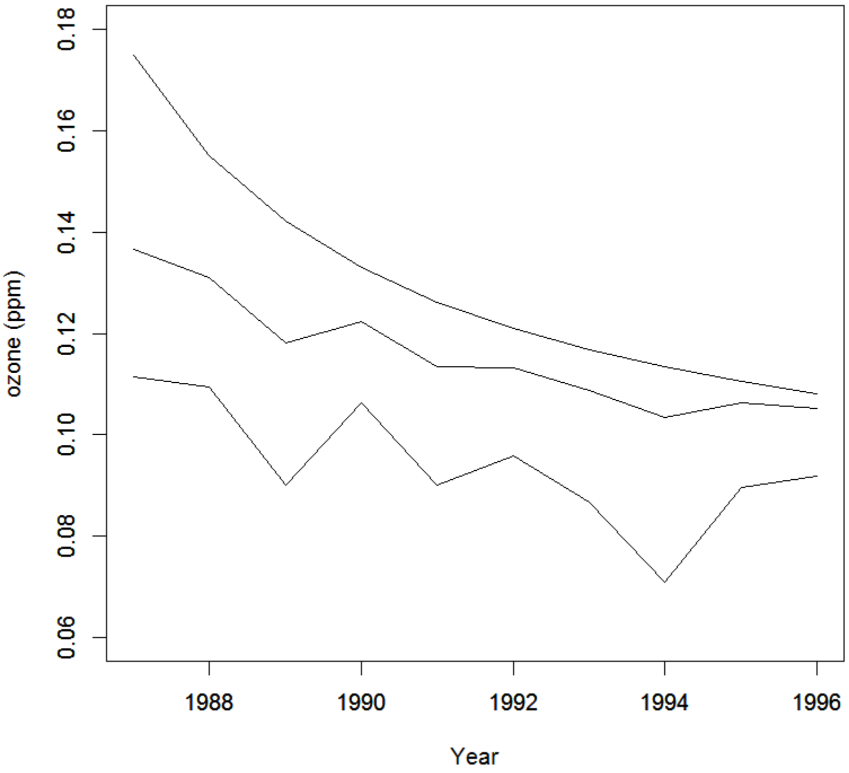

Figure 3: Estimated 0.99 and 0.999 quantiles, and estimated right endpoints of the distribution of ozone levels for a threshold of 0.08 ppm.

5. CONCLUSIONS

An exploratory data analysis of the extreme values of a time series of ozone levels made clear the existence of a decreasing linear trend in the size of the excesses over the threshold 8 ppm. We fitted the GPD to the POT's of the time series. By modeling the shape parameter of the GPD as a linear function of time in years, we were able to test the significance of a trend in the size of the excesses. More specifically, consider the years s and t with $s,t = 1987, ..., 1996$. Then we can say that the ozone excesses over 8 ppm for year s were more likely to take larger values then the ozone excesses over 8 ppm for year t, when $s < t$.

A. APPENDIX – Maximum Likelihood Calculations

The density function of a GPD(ξ,β) is

$$f(x;\xi,\beta) = \begin{cases} (1/\beta)\,(1-\xi x/\beta)^{(1/\xi)-1}\,, & \xi \neq 0\,,\ \beta > 0\,, \\ (1/\beta)\exp(-x/\beta)\,, & \xi = 0\,,\ \beta > 0\,. \end{cases}$$

Let $X_j \sim \text{GPD}(\xi_j,\beta)$, and let $x_j = (x_{1j}, ..., x_{n_j j})'$ be a random sample from X_j, $(j = 1, ..., k)$. Write $\xi_j = \xi + \theta t_j$. Then the log-likelihood function under $H_0\colon\ \theta = 0$ is

$$\text{(A.1)} \qquad l(\xi,\beta) \;=\; \sum_{j=1}^{k}\sum_{i=1}^{n_j} \log f(x_{ij};\xi,\beta) \;=\; -n\log\beta + (\xi^{-1}-1)\sum_{j=1}^{k}\sum_{i=1}^{n_j}\log(1-\xi x_{ij}/\beta)\,,$$

where $n = \sum_{j=1}^{k} n_j$, $(\xi,\beta) \in \Theta_0 = \big\{(\xi,\beta)\colon\ \xi<0,\ \beta>0\big\} \cup \big\{(\xi,\beta)\colon\ \xi>0,\ \beta>0, \text{ and } \beta/\xi > \max_{ij}(x_{ij})\big\}$. Making the reparametrization $(\xi,\beta) \mapsto (\xi,\tau)$, where $\tau = \xi/\beta$, the log-likelihood function becomes

$$l(\xi,\tau) \;=\; -n\log\xi + n\log\tau + (\xi^{-1}-1)\sum_{j=1}^{k}\sum_{i=1}^{n_j}\log(1-\tau x_{ij})\,,$$

where $\big\{\xi<0,\ \tau>0\big\} \cup \big\{0<\xi\le 1,\ \tau<1/\max_{ij}(x_{ij})\big\}$. The log-likelihood equations are

$$\text{(A.2)} \qquad \frac{\partial l}{\partial \xi} \;=\; (n/\xi) - (1/\xi^2)\sum_{j=1}^{k}\sum_{i=1}^{n_j}\log(1-\tau x_{ij}) \;=\; 0\,,$$

$$\text{(A.3)} \qquad \frac{\partial l}{\partial \tau} \;=\; (n/\tau) - (\xi^{-1}-1)\sum_{j=1}^{k}\sum_{i=1}^{n_j}\frac{x_{ij}}{1-\tau x_{ij}} \;=\; 0\,.$$

Solving equation (A.2) for ξ we obtain

$$\text{(A.4)} \qquad \xi(\tau) \;=\; -(1/n)\sum_{j=1}^{k}\sum_{i=1}^{n_j}\log(1-\tau x_{ij})\,.$$

Since equation (A.4) gives ξ as an explicit function of τ, we can substitute $\xi(\tau)$ of (A.4) in equation (A.3), and obtain

$$(n/\tau) - \big(\xi(\tau)^{-1} - 1\big) \sum_{j=1}^{k} \sum_{i=1}^{n_j} \frac{x_{ij}}{1 - \tau x_{ij}} = 0 \,,$$

which can be solved numerically for τ. If $\hat{\tau}$ is the solution, then the MLE's of ξ and β are given by $\hat{\xi} = \xi(\hat{\tau})$ and $\hat{\beta} = \hat{\xi}/\hat{\tau}$, respectively. This is the standard procedure to find the MLE's of the parameters of the GPD. For a detailed analysis of this procedure see Grimshaw [10]. Under $H_a\colon\ \theta > 0$ the log-likelihood function is

$$\begin{aligned} l(\xi,\theta,\beta) &= \sum_{j=1}^{k} \sum_{i=1}^{n_j} \log f(x_{ij};\xi,\theta,\beta) \\ &= -n \log\beta + \sum_{j=1}^{k} \big[(\xi+\theta t_j)^{-1} - 1\big] \sum_{i=1}^{n_j} \log\big[1 - (\xi+\theta t_j)\, x_{ij}/\beta\big] \,, \end{aligned}$$

where $(\xi,\theta,\beta) \in \Theta_a = \big\{(\xi,\theta,\beta)\colon \xi + \theta t_j < 0,\ j = 1, ..., k,\ \beta > 0,\ \theta > 0\big\} \cup \big\{(\xi,\theta,\beta)\colon \xi + \theta t_j > 0,\ j = 1, ..., k,\ \beta > 0,\ \theta > 0$ and $\beta/(\xi + \theta t_j) > \max_i(x_{ij}),\ j = 1, ..., k\big\}$. Let $x_{(n_j)j} = \max_i(x_{ij})$, and note that the restriction $\beta/(\xi+\theta t_j) > x_{(n_j)j}$ is equivalent to $\beta - \xi x_{(n_j)j} - \theta x_{(n_j)j} t_j > 0$. So, the parameter space $\Theta_a \subset \mathbb{R}^3$ is given by all the $(\beta,\xi,\theta)'$ that satisfy the linear pointwise restrictions

$$\begin{bmatrix} 1 & -x_{(n_1)1} & -x_{(n_1)1}t_1 \\ 1 & -x_{(n_2)2} & -x_{(n_2)2}t_2 \\ \vdots & \vdots & \vdots \\ 1 & -x_{(n_k)k} & -x_{(n_k)k}t_k \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \beta \\ \xi \\ \theta \end{bmatrix} > \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix} .$$

Finding the MLE's of ξ, θ, and β becomes a problem of maximization with linear constraints. There are several numerical algorithms to deal with this type of problem. In this work we used the Price's controlled random search procedure. See Khuri [13], pp. 334–336, for the details of this algorithm. The calculations were performed with R. The test statistic is given by $-2\log\lambda(x) = 2\big[l(\hat{\xi},\hat{\theta},\hat{\beta}) - l(\hat{\xi},\hat{\beta})\big]$.

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ROBUST ESTIMATION OF REDUCED RANK MODELS TO LARGE SPATIAL DATASETS

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Abstract:

- For large datasets, spatial covariances are often modeled using basis functions and covariance of a reduced dimensional latent spatial process. For skewed data, likelihood based approaches with Gaussian assumption may not lead to faithful inference. Any L_2 norm based estimation is susceptible to long tails and outliers due to contamination. Our method is based on an empirical binned covariance matrix using the median absolute deviation and minimizes L_1 norm between empirical covariance and the model covariance. The consistency of the proposed estimate is established theoretically. The improvement is demonstrated using simulated data and cloud data obtained from NASA's Terra satellite.

Key-Words:

- *geostatistics; contaminated data; median absolute deviation; quantile regression; cloud.*

1. INTRODUCTION

Analysis of geostatistical data is known to be computationally intense or infeasible when the number of observed locations, n, is large. This is due to the size of the covariance matrix, $\mathbf{\Sigma}$ (which is $n \times n$) and the computational demand of inverting or factoring it. Cressie and Johannesson [4] introduced Fixed Rank Kriging (FRK) to address the computational hurdle by modeling the spatial covariance through a fixed number of deterministic basis functions and a latent reduced rank spatial process. To introduce the parameters, we consider an observed spatial process $Z(\mathbf{s})$ to be made up of a hidden spatial process $Y(\mathbf{s})$ along with a white noise process $\varepsilon(\mathbf{s})$ which could represent, for example, measurement errors. So we write

$$Z(\mathbf{s}) = Y(\mathbf{s}) + \varepsilon(\mathbf{s})\,. \tag{1.1}$$

Typically $Y(\mathbf{s})$ and $\varepsilon(\mathbf{s})$ are assumed to be independent Gaussian distributions, with $\varepsilon(\mathbf{s})$ having mean of zero. In this work however we develop methods that are robust to departure from this assumption. Then, for n observed locations, $Z(\mathbf{s}) \equiv \big\{Z(\mathbf{s}_1), ..., Z(\mathbf{s}_n)\big\}$ is an n-dimensional process with mean $E(Y(\mathbf{s})) = \boldsymbol{\mu}_Y$ and covariance matrix expressed as $\mathbf{\Sigma}_Z = \mathbf{\Sigma}_Y + \sigma^2 \mathbf{I}_n$, where $\mathbf{\Sigma}_Y$ is the covariance matrix of $Y(\mathbf{s}) \equiv \big\{Y(\mathbf{s}_1), ..., Y(\mathbf{s}_n)\big\}$ and $\mathbf{I}_n$ is the identity matrix of rank n. We then model $Y(\mathbf{s})$ using a mixed effects model such as

$$Y(\mathbf{s}) = \mathbf{X}(\mathbf{s})\boldsymbol{\beta} + \mathbf{S}(\mathbf{s})\boldsymbol{\eta} + \delta(\mathbf{s})\,. \tag{1.2}$$

In this model $\mathbf{X}(\mathbf{s})$ is a matrix of known covariates and $\boldsymbol{\beta}$ is the associated vector of regression coefficients; $\mathbf{S}(\mathbf{s})$ is a sparse $n \times r$ matrix of fixed, spatially varying basis functions which are centered at a set of r knot locations. Dimension reduction is achieved by selecting $r \ll n$. Various classes of basis functions may be used, including wavelets (Shi and Cressie [18] and Zhu *et al.* [22]) and bisquare (Cressie and Johannesson [4] and Paul *et al.* [16]) functions. The latent process $\boldsymbol{\eta}$ is a zero-mean r-dimensional Gaussian process defined over the knot locations, with covariance matrix $\mathbf{V}$. Finally $\delta(\mathbf{s})$, the process error, is an *iid* zero-mean Gaussian process with variance τ^2 which takes into account the variations unexplained by the large scale variations $\mathbf{X}(\mathbf{s})\boldsymbol{\beta}$ and spatial process $\mathbf{S}(\mathbf{s})\boldsymbol{\eta}$, and uncertainties arising from the dimension reduction. The process and measurement errors are usually assumed to be independent. When there is only one observation at each spatial location, τ^2 and σ^2 are non-identifiable, instead their sum $\nu^2 = \sigma^2 + \tau^2$, called the nugget variance, is estimated (though indirect means exist to estimate these separately, see Katzfuss and Cressie [11]). Going forward, we suppress the dependence on $\mathbf{s}$ when possible by stacking scalers into vectors, and vectors into matrices (e.g., $Y(\mathbf{s})$ is replaced with $\mathbf{Y}$ and $\mathbf{X}(\mathbf{s})$ is replaced with $\mathbf{X}$).

With this framework, the covariance matrix $\mathbf{\Sigma}_Z$ can be written as $\mathbf{\Sigma}_Z = \mathbf{SVS}' + \nu^2 \mathbf{I}_n$. The objective is to estimate the model parameters: $\boldsymbol{\beta}, \mathbf{V}$ and ν^2. Once this has been done one may obtain the inverse of $\mathbf{\Sigma}_Z$ easily using the Sherman–Morrison–Woodbury matrix identity. This model offers a large degree of flexibility. The only restriction on $\mathbf{V}$ is the positive-definiteness, hence the resulting covariance matrix may be both anisotropic and nonstationary.

A variety of approaches have been used to model or estimate $\mathbf{V}$. In introducing FRK, Cressie and Johannesson [4] used a Method of Moments (MoM) estimation scheme, while Katzfuss and Cressie [11] developed an expectation-maximization (EM) algorithm. Much attention has also been given to Bayesian hierarchical modeling (see, for example, Banerjee *et al.* [1], Kang *et al.* [9] and Kang and Cressie [8]). To-date, little attention appears to have been given to robust estimation schemes. Zhu *et al.* [22] developed a method to reduce bias through improved basis function selection, but otherwise did not consider distributional assumptions. Paul *et al.* [16] developed a scale mixture model applicable to non-Gaussian datasets, but like many Bayesian methods it can be time-intensive to implement and run.

The basic FRK model we have described has been elaborated in various ways. For example, to obtain better representation of the spatial dependence some have used a tapering approach (Sang and Huang [17]) or multiple sets of knot locations with different resolutions (Cressie and Johannesson [4] and Kang *et al.* [10]). We demonstrate the latter approach in our data application in Section 5. Both the estimation and fitting stages in the existing MoM estimation use least-squares concepts, and therefore may suffer in the presence of skewed or contaminated data. In the present work we develop an alternative MoM estimator for the parameters of the RRSM. Our motivation in this is to provide an estimator that can model data containing outliers or exhibiting skewness, two features that are frequently encountered in geostatistical datasets, and which does not require significant computational resources.

MoM estimation of the model parameters is divided into two stages: an estimation stage and a fitting stage. In the estimation stage, the entire spatial domain is divided into M bins such that $r < M \ll n$, and $\boldsymbol{\Sigma}_M$ is defined to be the covariance matrix over the bins. The bins are defined subjectively, though Cressie and Johannesson [4] and Katzfuss and Cressie [11] provide some recommendations. Then an empirical estimate $\hat{\boldsymbol{\Sigma}}_M$ is constructed using the *detail residuals*, $\mathbf{D} = \mathbf{Z} - \mathbf{X}\hat{\boldsymbol{\beta}}$, where $\hat{\boldsymbol{\beta}}$ is the ordinary least squares estimate of $\boldsymbol{\beta}$. Cressie and Johannesson [4] defined $\hat{\boldsymbol{\Sigma}}_M$ in the following manner: The m^{th} diagonal elements $\hat{\boldsymbol{\Sigma}}_M(m,m) = \text{avg}(\mathbf{D}_m^2)$ and the (m,m') off-diagonal element $\hat{\boldsymbol{\Sigma}}_M(m,m') = \text{avg}(\mathbf{D}_m) \times \text{avg}(\mathbf{D}_{m'})$. In these expressions, $\mathbf{D}_m$ is the vector of detail residuals in bin m, and $\text{avg}(\cdot)$ denotes the average.

Similarly $\mathbf{S}$ is binned into an $M \times r$ matrix by taking the column averages of the rows of $\mathbf{S}$ associated with the observed locations falling into each of the M bins. Denoting this as $\overline{\mathbf{S}}$, one may then write

$$\boldsymbol{\Sigma}_M = \overline{\mathbf{S}}\mathbf{V}\overline{\mathbf{S}}' + \nu^2\mathbf{I}_M\,. \tag{1.3}$$

After estimation, the fitting stage obtains $\hat{\mathbf{V}}$ and $\hat{\nu}^2$ by minimizing the Frobenius norm between $\boldsymbol{\Sigma}_M$ and $\hat{\boldsymbol{\Sigma}}_M$, using the QR-decomposition on $\overline{\mathbf{S}}$. This is a two-step process resulting in the following estimates:

$$\begin{aligned}\hat{\nu}^2 &= (\mathbf{F}'\mathbf{F})^{-1}\mathbf{F}'\big(\hat{\boldsymbol{\Sigma}}_M - \mathbf{Q}\mathbf{Q}'\hat{\boldsymbol{\Sigma}}_M\mathbf{Q}\mathbf{Q}'\big)\,,\\ \hat{\mathbf{V}} &= \mathbf{R}^{-1}\mathbf{Q}'\big(\hat{\boldsymbol{\Sigma}}_M - \hat{\nu}^2\mathbf{I}_M\big)\mathbf{Q}\mathbf{R}'^{-1}\,,\end{aligned}$$

where $\mathbf{F} = \mathbf{I}_M - \mathbf{Q}\mathbf{Q}'$. If $\hat{\boldsymbol{\Sigma}}_M$ is not positive-definite, the eigenvalues must be lifted to ensure that $\hat{\mathbf{V}}$ is positive-definite (see Kang *et al.* [9]). For further details on Fixed Rank Kriging, see Katzfuss and Cressie [11].

We redesign both the estimation and fitting stages for the MoM estimation using the Median Absolute Deviation and quantile regression (Section 2). Our work is novel in that we return to basic principles to redesign the estimation and fitting stages with a mind for resisting contaminated data. The consistency of our proposed estimate is shown (Section 3), though the technical details are given in the Appendix. We describe and conduct a simulation study (Section 4) to investigate the performance of our proposed method. Finally, we provide a data example (Section 5) using a large remote sensing dataset and some concluding remarks (Section 6).

2. ROBUST ESTIMATION AND FITTING

In this section we describe robust alternatives to both the estimation stage and fitting stage of MoM estimation for the FRK model. First we define $\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}$ as an estimate empirical binned covariance matrix which is robust to contamination. Then we describe a robust strategy to fit the model parameters, which we call the *robust fit*. We denote the previous-described methods from Cressie and Johannesson [4] as $\hat{\mathbf{\Sigma}}_M^{(\mathrm{CJ})}$ and the Frobenius fit.

2.1. Estimation stage

The diagonal elements of $\mathbf{\Sigma}_M$ represent the variance within a bin. We estimate this quantity using the median absolute deviation, $\mathrm{MAD}(X) = \mathrm{med}\big(|X - \mathrm{med}(X)|\big)$. A constant scale factor is applied to the MAD which causes it to be a consistent estimate for the standard deviation (see Hettmansperger and McKean [7], Eqn. 3.9.27). In the present work, we use the usual MAD which is consistent for σ when the errors are normally distributed. Hence, the diagonal elements of our proposed estimate are given by

$$\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}(m,m) = \mathrm{MAD}^2(\mathbf{D}_m)\,, \qquad m = 1, ..., M\,. \tag{2.1}$$

Estimating the covariance between two bins is more challenging. First, recall that $\mathrm{cov}(A,B) = \frac{1}{4}\big[V(A+B) - V(A-B)\big]$. Estimating a covariance using this identity requires finding $\mathbf{D}_m \pm \mathbf{D}_{m'}$, however, these quantities are not well-defined. For example, two bins may not even have the same number of observations, much less any natural correspondence between observations. We therefore use the pairwise sums and pairwise differences, denoted using $\oplus$ and $\ominus$ respectively, to approximate $\mathbf{D}_m \pm \mathbf{D}_{m'}$. We again use the square of the MAD to estimate the variance, so the off-diagonal elements of our estimate are given by:

$$\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}(m,m') \;=\; \frac{1}{4}\Big[\mathrm{MAD}^2(\mathbf{D}_m \oplus \mathbf{D}_{m'}) - \mathrm{MAD}^2(\mathbf{D}_m \ominus \mathbf{D}_{m'})\Big]. \tag{2.2}$$

2.2. Fitting stage

Given an empirical covariance matrix $\hat{\mathbf{\Sigma}}_M$, we fit $\mathbf{V}$ by minimizing some norm between $\hat{\mathbf{\Sigma}}_M$ and $\mathbf{\Sigma}_M$. To develop the robust fitting stage, we start from equation (1.3),

$$\begin{aligned} \hat{\mathbf{\Sigma}}_M &= \overline{\mathbf{S}}\mathbf{V}\overline{\mathbf{S}}' + \hat{\nu}^2\mathbf{I}_M\,, \\ \big(\hat{\mathbf{\Sigma}}_M - \hat{\nu}^2\mathbf{I}_M\big)\,\overline{\mathbf{S}}\big(\overline{\mathbf{S}}'\overline{\mathbf{S}}\big)^{-1} &= \overline{\mathbf{S}}\mathbf{V}. \end{aligned} \tag{2.3}$$

Then we may see equation (2.3) as a multivariate regression problem with $\overline{\mathbf{S}}$ as the design matrix and $\mathbf{V}$ as the matrix of regression coefficients. Any method of robust regression may then be implemented to obtain an estimate of $\mathbf{V}$. For this work, we use the popular least absolute deviations, L_1, estimator; see Koenker and Bassett [13] and Section 3.8 of Hettmansperger and McKean [7]. In comparison to least squares (LS), the least absolute deviation fit is obtained by replacing the squared Euclidean norm with the L_1 norm. Hence, the geometry and interpretation of the L_1 fit is quite similar to LS fit, but unlike the LS estimate, the L_1 estimate is robust. As discussed in Section 3.8 of Hettmansperger and McKean [7], the fit is also efficient. It attains efficiency 0.64 relative to LS for normal errors but is generally more efficient than LS for error distributions with tails heavier than the normal.

Each column of $\left(\hat{\mathbf{\Sigma}}_M - \hat{\nu}^2\mathbf{I}_M\right)\overline{\mathbf{S}}\left(\overline{\mathbf{S}}'\overline{\mathbf{S}}\right)^{-1}$ is used as the response in a separate estimation. There are therefore r estimates to obtain, each of which corresponds to a column of $\mathbf{V}$. As the final estimate $\mathbf{V}$ may not be numerically symmetric, we symmetrize $\hat{\mathbf{V}}$ by taking $\hat{\mathbf{V}} = 0.5\left(\hat{\mathbf{V}} + \hat{\mathbf{V}}'\right)$. We used the `quantreg` `R` package (Koenker [12]) for the computation of the L_1 fit.

Estimation of $\mathbf{V}$ requires an estimate of ν^2. By substituting the left side of (2.3) for $\overline{\mathbf{S}}\mathbf{V}$ in (1.3) we obtain:

$$\hat{\mathbf{\Sigma}}_M = \left(\hat{\mathbf{\Sigma}}_M - \nu^2\mathbf{I}_M\right)\overline{\mathbf{S}}\left(\overline{\mathbf{S}}'\overline{\mathbf{S}}\right)^{-1}\overline{\mathbf{S}}' + \nu^2\mathbf{I}_M\,,$$

$$\hat{\mathbf{\Sigma}}_M\Big(\mathbf{I}_M - \overline{\mathbf{S}}\left(\overline{\mathbf{S}}'\overline{\mathbf{S}}\right)^{-1}\overline{\mathbf{S}}'\Big) = \nu^2\Big(\mathbf{I}_M - \overline{\mathbf{S}}\left(\overline{\mathbf{S}}'\overline{\mathbf{S}}\right)^{-1}\overline{\mathbf{S}}'\Big)\,. \tag{2.4}$$

We then stack the columns of $\hat{\mathbf{\Sigma}}_M\left(\mathbf{I}_M - \overline{\mathbf{S}}\left(\overline{\mathbf{S}}'\overline{\mathbf{S}}\right)^{-1}\overline{\mathbf{S}}'\right)$ and the columns of $\left(\mathbf{I}_M - \overline{\mathbf{S}}\left(\overline{\mathbf{S}}'\overline{\mathbf{S}}\right)^{-1}\overline{\mathbf{S}}'\right)$. Doing this, we again cast the problem as a zero-intercept robust regression, where ν^2 is the slope. This estimate is substituted into equation (2.3) to obtain an estimate of $\mathbf{V}$.

The estimate of $\mathbf{V}$ may not be positive-definite, so we may need to lift the eigenvalues (similar to Cressie and Johannesson [4]), while preserving the total variability. In our work, we compute the sum of the eigenvalues, Δ, and proportionally redistribute this sum across the eigenvalues after shifting all eigenvalues to be non-negative.

3. ASYMPTOTIC PROPERTIES

Here we discuss some of the infill asymptotic properties of our proposed estimator, $\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}$. Infill asymptotics is a common method of considering asymptotics related to geostatistical methodology in which the domain, $\mathcal{D}$, remains fixed but the density of observed locations is increased.

Recall that we obtain $\hat{\mathbf{V}}$ by minimizing some norm $\|\cdot\|$:

$$\hat{\mathbf{V}} = \operatorname{argmin}\left\|\hat{\mathbf{\Sigma}}_M - \mathbf{\Sigma}_M\right\|.$$

Hence, once $\hat{\mathbf{\Sigma}}_M$ is known, $\hat{\mathbf{V}}$ is fully determined by the fitting method. Therefore, a desirable property of the empirical binned covariance matrix $\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}$ is that it be consistent for $\mathbf{\Sigma}_M$, which we establish in this section.

There are two sets of assumptions that we need to make. From expressions (2.1) and (2.2), $\hat{\boldsymbol{\Sigma}}_M^{(\mathrm{rob})}$ is a function of MADs applied to the detail residuals. For each bin m, these residuals are obtained from ordinary least-squares regression, our proof requires that $\sqrt{n}\,(\hat{\beta}-\beta) = O(1)$ for each bin. For this, we assume the conditions in the paper by Lahiri *et al.* [14] for each bin.

Our process for bin j (slightly abusing the notation to avoid double subscript), is $\{e_1, e_2, ..., e_{n_j}\}$ which we denote by $\{\mathbf{e}_j\}$. On this process we assume that

1. $\{\mathbf{e}_j\}$ is stationary.

2. $\{\mathbf{e}_j\}$ satisfies the strong mixing coefficients assumption given as follows. For $i \neq k$, let A_i and B_k be in the σ-fields generated by e_i and e_k. Then

$$\Big|P[A_i \cap B_k] - P[A_i]\,P[B_k]\Big| = O\big(\rho^{|i-k|}\big)\,, \tag{3.1}$$

where $0 \leq \rho < 1$.

Note that Assumption 2 implies that the spatial correlation between two locations exhibits exponential decay. This is a common feature in spatial modeling (e.g. the Matérn class of covariance models), and as such is not an unreasonable assumption.

For our proof, let $\mathbf{D}_m$ denote the random detail residual process within the m^{th} bin, and let $\mathbf{D}_m = \{\tilde{R}_{m_1}, ..., \tilde{R}_{m_k}\}$ be the k observed detail residuals from that bin. We assume that $\mathbf{D}_m$ and, as will be seen, $|\mathbf{D}_m|$, exhibit strong mixing as described in conditions 1 and 2.

We now state the consistency result in theorem form. The proof is given in the Appendix.

Theorem 3.1. *Under the above conditions,* $\hat{\boldsymbol{\Sigma}}_M^{(\mathrm{rob})}$ *is a consistent estimator of* $\boldsymbol{\Sigma}_M$*.*

Throughout we treat the number of bins, M, as fixed, and do not consider limits over that quantity. This is analogous to the work of Bliznyuk *et al.* [2]. In another context on binned estimation, they considered m (the number of bins) as a radius to determine "adjacency" of locations, where m does not depend on n, (the number of observations) and did not limit over m. The only restriction on M is that it should be large enough to ensure that the assumption of stationary within bins holds for practical implementation.

4. SIMULATION STUDY

To compare our proposed methods with the existing methods using simulated data, we generate a spatial process Z according to the model:

$$\mathbf{Z} = \mathbf{X}\boldsymbol{\beta} + \mathbf{S}\boldsymbol{\eta} + \boldsymbol{\epsilon}\,.$$

First we select n locations uniformly over a 100×100 domain, and $r_o = 1225$ knot locations on a 35×35 grid. These knot locations are used to simulate the data but not to fit the models (because reduced rank spatial models are designed as approximations of a more complex spatial process). Then we define $\mathbf{X}$ as an $n\times3$ matrix where the columns correspond respectively to an intercept, the x-coordinate, and the y-coordinate.

To define $\mathbf{V}$ we first compute the pairwise distances between the knot locations, and generate a Matérn covariance matrix using these distances with sill and range parameters each set to 1, and smoothness set to 0.5. We use `cov.sp` in the `R` package `SpatialTools` (French [6]) to generate this matrix. We then obtain $\mathbf{V}$ as an observation from the inverse Wishart distribution using the Matérn covariance as a scale matrix and $2(r+1)$ degrees of freedom. In this way the covariance matrix used to simulate the data is not constrained to be either stationary or isotropic.

We construct $\mathbf{S}$ using the bisquare basis functions defined as

$$S_{i,j} = \begin{cases} \left(1 - \left(\|s_i - u_j\|/r_u\right)^2\right)^2 & \text{for } \|s_i - u_j\| \leq r_u\,, \\ 0 & \text{otherwise}\,, \end{cases}$$

where r_u is 1.5 times the minimum distance between knots and $\|\cdot\|$ denotes the measure of distance appropriate to the data (e.g., in our simulations, we used Euclidean distance).

We used two methods to simulate the data, a Contaminated Normal distribution and an Exponential distribution. These simulate the presence of outliers or of skewness, respectively, in the resulting dataset. For either simulation method, we compare the model fits by splitting the simulated data into a training set and a held-out test set. The hold-out set was set as all of the locations in the square bounded by the points $(40, 40)$ and $(60, 60)$, which corresponds to approximately 4% of the observations. We use the estimated parameters to predict at the held-out locations and compute diagnostics to assess both the accuracy and uncertainty of the prediction, including the mean square error (MSE), mean square prediction error (MSPE), and the continuous ranked probability score (CRPS, Wilks [21]), a measure which incorporates both the prediction accuracy and the prediction uncertainty. Lower values are preferable for all of these measures.

4.1. Simulation 1: contaminated normal

For simulating datasets we first generate a r_o-dimensional process $\boldsymbol{\eta}$ from a zero-mean multivariate normal with covariance $\mathbf{V}$. To induce outliers, the measurement error process $\boldsymbol{\varepsilon}$ is generated from a contaminated normal distribution. We first draw a random sample from $\mathcal{N}(0, \nu^2)$, and then replace αn of the values with random draws from $\mathcal{N}(0, \nu_c^2)$. Finally, we obtain the simulated data by $\mathbf{Z} = \mathbf{X}\boldsymbol{\beta} + \mathbf{S}\boldsymbol{\eta} + \boldsymbol{\varepsilon}$. For each simulated dataset, estimate model parameters using both the method of Cressie and Johannesson [4] and the proposed robust method.

We considered three sample sizes, $n \in \{10000, 15000, 20000\}$ and five levels for the number of knots locations to fit the model, $r \in \{64, 100, 144, 196, 256\}$, intentionally chosen to much less than r_o, so that the "true" spatial process was more granular than the model. For the contamination level of $\boldsymbol{\varepsilon}$ we consider $\alpha \in \{0.00, 0.05, 0.10, 0.15, 0.20\}$. For the simulations shown, the values of $\boldsymbol{\beta} = (1, 0.01, 0.05)'$, $\nu^2 = 1$, and $\nu_c^2 = 100$ were held constant. These choices are not sensitive to our estimation technique except insofar as a larger or smaller ν_c^2 would correspond to a larger or smaller effect from the contamination. For each combination of these parameters, we generated 50 replications of data. Hence, there were 75 settings of parameter levels, and 3750 replications in total.

4.2. Simulation 2: exponential

As we have noted throughout, skewness can also be problematic for least-squares type estimators, and skewed data are not uncommon in geostatistics. Hence, we designed a second simulation in which we generate $\boldsymbol{\varepsilon}$ from an Exponential distribution rather than from a contaminated Normal distribution. We use the same design as Simulation 1, but instead of α, we consider the rate parameter of the Exponential distribution $\lambda \in \{0.10, 0.25, 0.50, 1.00\}$. Hence, for this simulation there were 60 settings and 3000 replications in total.

4.3. Simulation results

The simulations suggest that the robust method is generally preferable to the CJ method. For brevity we present the results for the CRPS, but results for the MSE and MSPE were similar. We use two main values to compare the results: The median CRPS across the 50 replications, and the CRPS of the CJ method relative to that of the robust method (we refer to this as the CRPS ratio).

Results of Simulation 1 are shown in Figure 1, which plots the median CRPS over the 50 replications for each of the settings. In 67 of the 75 settings, the robust method produced a smaller median CRPS than the CJ method.

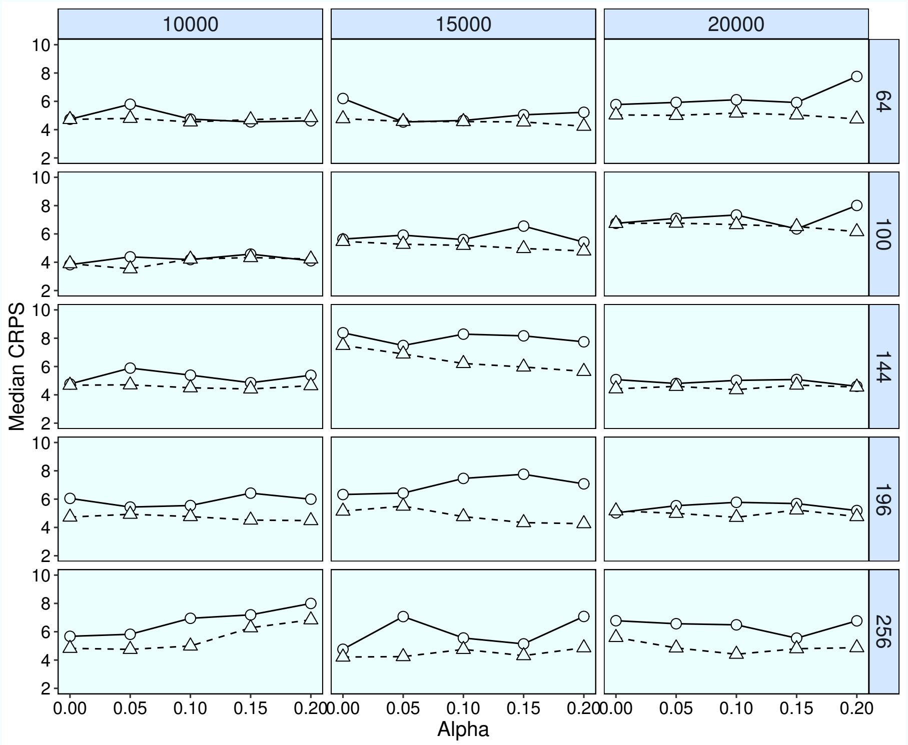

Figure 1: Results for Simulation 1. Plotted points are median CRPS of the CJ method (circles) and the robust method (triangles) over the 50 replications.

In addition, the robust method produced a smaller CRPS (i.e. CRPS ratio greater than 1) in 68.8% of the replications, and the median of the CRPS ratio showed a 9% larger CRPS for the CJ method. When considering the CRPS ratio for each setting, the worst-performing setting for the robust method had a median CPRS ratio of 0.975 (near equivalence), while half of the settings had a median CRPS ratio showing an improvement of 10% or more.

The results for Simulation 2 were similar to those of Simulation 1, and are shown in Figure 2. In 55 of the 75 settings, the robust method produced a smaller median CRPS than the CJ method.

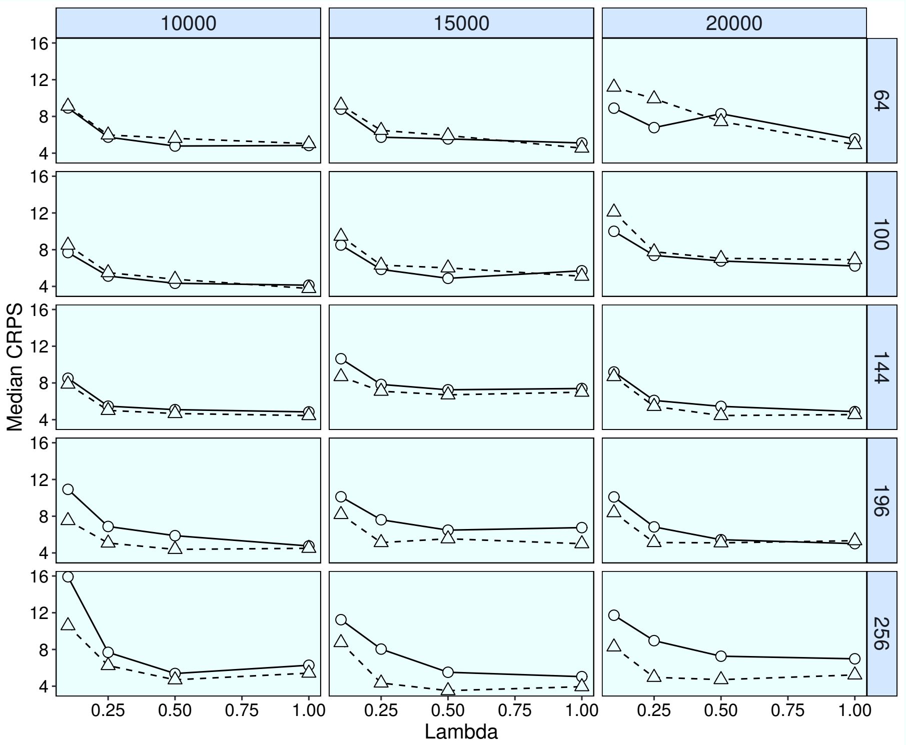

Figure 2: Results for Simulation 2. Plotted points are median CRPS of the CJ method (circles) and the robust method (triangles) over the 50 replications.

In addition, the robust method produced a smaller CRPS (i.e. CRPS ratio greater than 1) in 65.3% of the replications, and the median of the CRPS ratio showed an 8% larger CRPS for the CJ method. When considering the CRPS ratio for each setting, the worst-performing setting for the robust method had a median CPRS ratio of 0.957, which again shows minimal advantage for the CJ method, while half of the settings had a median CRPS ratio showing an improvement of at least 7%.

To provide an overall summary of our results, our findings suggest that the proposed robust method tends to be advantageous compared to the CJ method. While we acknowledge this is not uniformly the case, we note that in approximately two-thirds of cases, the proposed method resulted in smaller CRPS. It is unfortunately difficult to discern much in the way of a pattern across the simulation settings, to determine whether the robust or CJ method might be preferable in a specific setting. The main apparent pattern from these simulations is that the more knots, the better the robust method tended to perform against the CJ method.

This could potentially be a consequence of each bin from the estimation of $\boldsymbol{\Sigma}_M$ having fewer observations compared to a setting with the same sample size but smaller number of knots, in which case outliers would have an increased effect.

Since the number of knots is chosen by the modeler, one might be tempted to select a smaller value of r, so that any effect from the choice of method is minimized. However, fewer knots corresponds to a more coarse representation of the spatial variation, hence the general recommendation (e.g. Finley *et al.* [5]) is to use as many as possible (within any computational limits). Hence, the natural choice guiding the selection of r will also tend to produce situations in which the robust method appears to perform better.

5. APPLICATION TO NASA DATA

We use remote sensing data on daily cloud liquid water path (CWP), obtained through NASA's Moderate Resolution Imaging Spectroradiometer (MODIS) on the Terra satellite on April 22, 2012. Note that this date is an arbitrary choice, our interest here is to demonstrate our method outside of a fabricated example. Because the dataset is large ($n = 48552$), a reduced rank model is a reasonable choice for inference. The CWP data are right-skewed, so we restrict out focus to the log-scale.

5.1. Original Data Analysis

The observed data are plotted in Figure 3. Due to a north-south trend (tending to smaller values closer to the equator), we model the large-scale variation using Legendre polynomials similar to Stein [19], though using only the latitude. Specifically, let L denote the degrees latitudes and define $\ell = \pi(L/180)$.

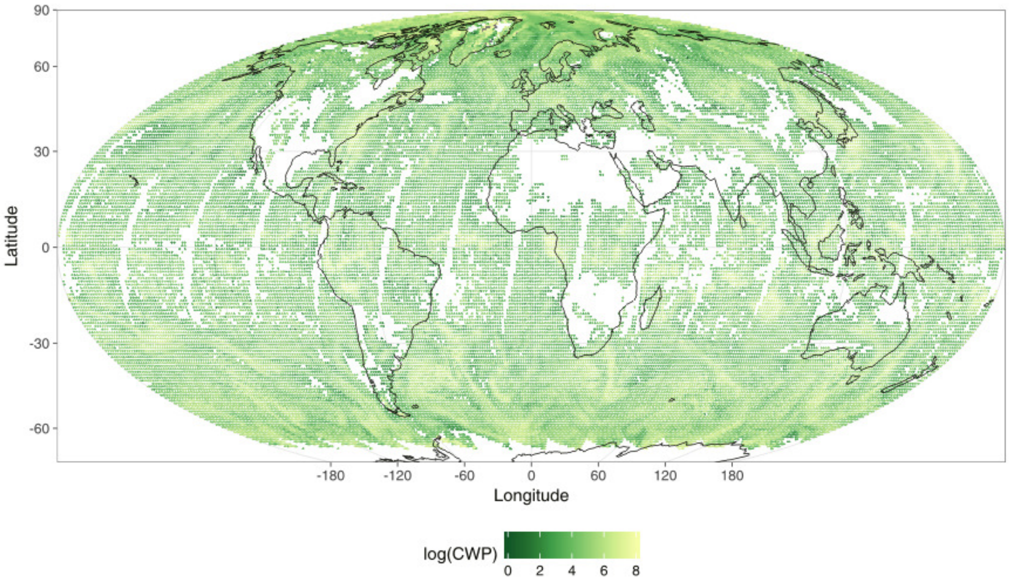

Figure 3: Plot of observed Cloud Water Path over the spatial domain.

We compute Legendre polynomials $P_p^q(\sin(\ell))$ of degree $p = 80$ and order $q = 0, 1, ..., p$. This results in a design matrix consisting of 81 regressors of spherical harmonics. Stein [19] also included a cosine of the longitude. Since we observed primarily a trend over the latitudes, we do not include the cosine term on longitude. Since our focus is on the small-scale (spatial) variation rather than the large-scale variation, the main concern for us is that this model enables stationarity of the spatial process to be reasonable; visual inspection (figure not shown) of the predictions for each latitude show this to be the case.

For the MoM estimation described in the preceding sections we first compute the detailed residuals. The normal quantile-quantile plot of the detailed residuals in Figure 4 shows a heavy lower tail, which motivates the use of the proposed robust techniques. Initially we model the data as observed. Afterwards, we also induce outliers into the data and reanalyze the data.

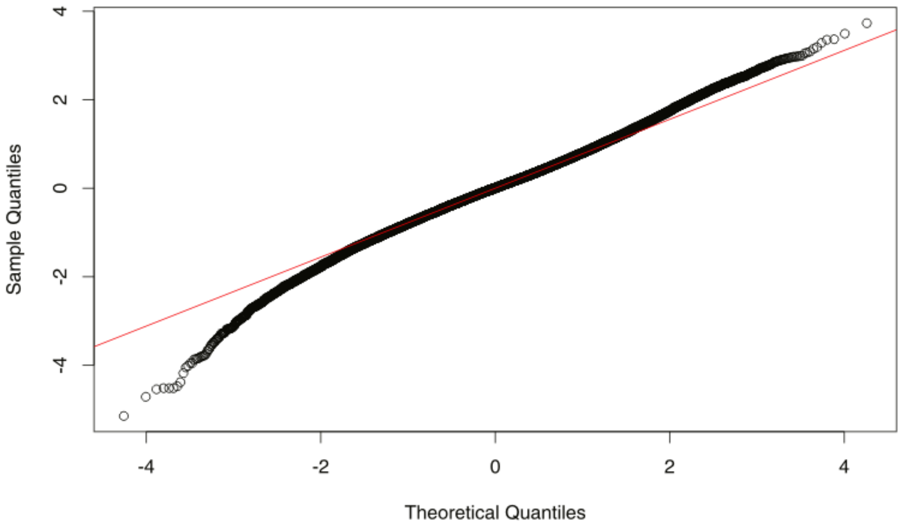

Figure 4: Normal quantile-quantile plot of the detailed residuals.

As recommended by Cressie and Johannesson [4], we use a multi-resolution model for CWP (see Nychka *et al.* [15]), to capture multiple scales of variation. We choose $r_1 = 38$ knot locations for the first resolution, and $r_2 = 97$ knot locations for the second resolution. Therefore the estimate of $\mathbf{V}$ is a 135×135 matrix. A map of these knot locations is given in Figure 5.

To construct the $\mathbf{S}$ matrix, we use the modified bisquare function, defined as:

$$\mathbf{S}_{i,j(l)} = \begin{cases} \left(1 - 0.25\, d^2\big(\mathbf{s}_i, \mathbf{u}_{j(l)}\big)\right) & \text{for } d\big(\mathbf{s}_i, \mathbf{u}_{j(l)}\big) \le 2\,, \\ 0 & \text{otherwise}\,, \end{cases}$$

where $\mathbf{u}_{j(l)}$ is the j^{th} knot location of the l^{th} resolution, $\mathbf{s}_i$ are the observed locations. The distance is given by:

$$d\big(\mathbf{s}_i, \mathbf{u}_{j(l)}\big) = \sqrt{d^2_{\text{long}}\big(\mathbf{s}_i, \mathbf{u}_{j(l)}\big)/r^2_{\text{long}(l)} + d^2_{\text{lat}}\big(\mathbf{s}_i, \mathbf{u}_{j(l)}\big)/r^2_{\text{lat}(l)}}\;,$$

where $d_{\text{long}}\big(\mathbf{s}_i, \mathbf{u}_{j(l)}\big)$ and $d_{\text{lat}}\big(\mathbf{s}_i, \mathbf{u}_{j(l)}\big)$ denote the longitude (east-west) and latitude (north-south) distances, respectively, between the location $\mathbf{s}$ and the knot location $\mathbf{u}_{j(l)}$. The values

$r_{\text{long}(l)}$ and $r_{\text{lat}(l)}$ control the maximum distance between an observation and a knot such that there is non-zero weight associated between the two. We set these to be the minimum east-west distance and minimum north-south distance between two knot locations of the same resolution.

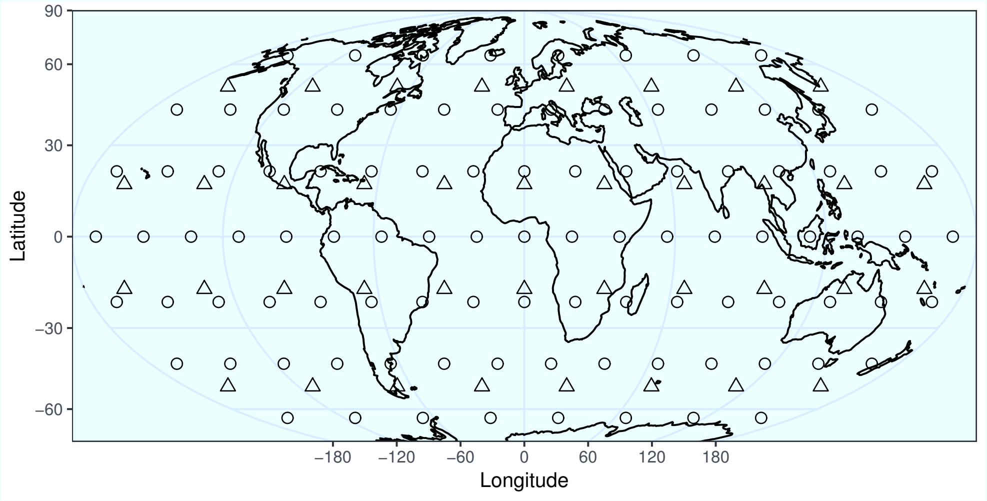

Figure 5: Plot of the knot locations of the basis functions over the spatial domain. Triangles represent the 38 knot locations of the first resolution, and circles represent the 97 knot locations of the second resolution.

Figures of the predictions or prediction uncertainties are not particularly informative, as our focus is on comparing the robust method to the CJ method. The CJ method yielded larger RMSPEs by approximately 20%, and the CRPS tended to be larger as well. A plot of the CRPS ratio for each location is shown in Figure 6. On average, the CRPS ratio is 1.04, indicating better performance for the robust method.

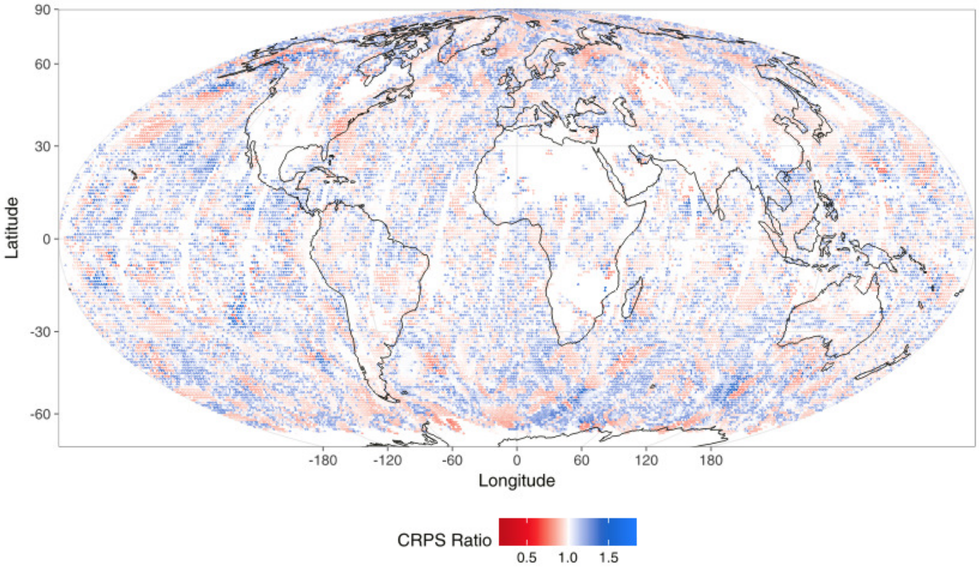

Figure 6: Plot of the CRPS of predictions using the CJ method relative to those using the robust method. Larger values indicate the CJ method produced a larger CRPS at that location.

5.2. Analysis after inducing outliers

In addition to this analysis, we artificially contaminated the log CWP data by replacing the 2% of observed values $Z_i(\mathbf{s})$ with $1.5\,Z_i(\mathbf{s})$. Inspection of the normal quantile-quantile plot showed a heavy upper tail which also contained many outliers. The results followed the same pattern as those described above. The RMSPE were again uniformly larger for the CJ method, now averaging 78% larger, while the CRPS were, on average, 11% larger.

6. CONCLUSIONS AND DISCUSSION

The Method of Moments is a flexible and powerful tool for estimating the parameters of a FRK model. Bayesian methods are more accurate than kriging (Kang and Cressie [8]), but they are also more time-consuming, and often come with some distributional assumptions. Kriging is typically a faster process, and kriging estimates are BLUP even in the face of non-normality, so kriging presents benefits of its own. However the typical parameter estimates using EM algorithm or MoM are susceptible to contaminated data. In this work we have provided robust alternatives to both stages of the MoM estimation.

Our results indicate that the proposed estimate and fitting scheme successfully capture the spatial covariance. In both our simulations and in our application to real data, the robust method tended to provide an advantage over the CJ method. At times the advantage was small, but in some cases the robust method showed substantial improvement, even when the data were neither contaminated or skewed.

Besides the L_1-fit, other robust fits can be used. For example, the Wilcoxon fit is a robust fit that minimizes the sum of the absolute differences of the residuals (see Hettmansperger and McKean [7], Section 3.8). The Wilcoxon fit is generally more efficient than the L_1-fit and it generalizes to fits for skewed-error distributions. We are currently investigating other robust norms which result in fits with higher efficiency than that of the L_1 fit for normal errors.

Again we emphasize that the kriging equations have been derived by minimizing the mean square prediction error. These predictions are then simply functions of $\mathbf{V}$ and ν. In our work, we have provided robust methods of estimating these same parameters. Yet when using robust techniques, it may be desirable to derive predictions and measures of precision using a different loss function than the squared error loss, or such that the predictions are robust in addition to the parameter estimates (Cressie and Hawkins [3]). Our robust estimates perform well in spite of this.

A. APPENDIX – Proof of Theorem 3.1

The proof utilizes the consistency of a fit $\hat{\beta}$ such that $\sqrt{n}\left(\hat{\beta}-\beta\right)=O(1)$; the assumptions as discussed in Section 3, including $n_j \to \infty$, for $j=1,...M$; and the theory for the sign processes as discussed in Chapters 1 and 3 of Hettmansperger and McKean [7]. For the sign process theory, we assume that the pdf of the random errors is positive at its median. The proof is in two parts. Part 2 gives the desired result, while Part 1 establishes the consistency of the medians used in the second part.

Part 1 of the Proof:

Consider the j-th bin, for $j=1,...M$. Let $\{\mathbf{e}_j\}$ denote the process of random errors of the linear model $\mathbf{Z}_j=\mathbf{X}_j\boldsymbol{\beta}_j+\mathbf{e}_j$. Assume without loss of generality that $\boldsymbol{\beta}_j=\mathbf{0}$ and the median of e_i is 0, where for ease of notation we have omitted the second subscript j on e_i. Let $\hat{\mathbf{e}}=\mathbf{Z}_j-\mathbf{X}_j\hat{\boldsymbol{\beta}}_{j,ls}$ denote the residuals from the a fit such that $\sqrt{n}\left(\hat{\beta}-\beta\right)=\mathcal{O}(1)$. Let $F(t)$ and $f(t)$ denote the cdf and pdf of e_i, respectively.

Consider the sign process given by

$$\overline{S}_j(\theta)=\frac{1}{n_j}\sum_{i=1}^{n_j}\operatorname{sgn}(e_i-\theta)\,, \tag{A.1}$$

where $\operatorname{sgn}(u)=-1,0,\text{or }1$ for $u<0$, $u=0$, or $u>0$. Denote the median of $e_1,...,e_{n_j}$ by $\hat{\theta}_e$. Notice that $\hat{\theta}_e$ solves the equation $\overline{S}_j(\theta)=0$. Our immediate goal is the asymptotic linearity of the process $\overline{S}_j(\theta)$ that is given in expression (A.3). We accomplish this by showing that the four sufficient conditions hold as given in Section 1.5 of Hettmansperger and McKean [7]. First note that $\overline{S}_j(\theta)$ is a nonincreasing function of θ. Thus the first condition holds. For the second condition, by a simple shift theorem and stationarity, we have

$$\mu(\theta)\,=\,E_0\big[\overline{S}_j(\theta)\big]\,=\,E_\theta\big[\overline{S}_j(0)\big]\,=\,\frac{1}{n_j}\sum_{i=1}^{n_j}E_\theta\big[\operatorname{sgn}(e_i)\big]\,=\,1-2F(-\theta)\,.$$

Hence, $\mu'(0)=2f(0)>0$ which establishes the second condition.

For the third condition, we need to show the variance of $\sqrt{n_j}\,\overline{S}_j(0)$ exists. This variance is

$$\begin{aligned}\sigma^2_{n_j}&=V\big[\sqrt{n_j}\,\overline{S}_j(0)\big]\\&=\frac{1}{n_j}\sum_{i=1}^{n_j}V\big(\operatorname{sgn}(e_i)\big)+\frac{2}{n_j}\sum_{i=1}^{n_j-1}\sum_{k=i+1}^{n_j}\operatorname{cov}\big[\operatorname{sgn}(e_i),\operatorname{sgn}(e_k)\big]\,.\end{aligned}$$

The first term on the right is easily seen to be 1. Using $P[e_i<0]=1/2$ and expanding each covariance term into its expectation, we obtain four probability terms and, hence, the sum of four series. The absolute value of one of these four series is given next. As we show, we establish a bound on the series by invoking the assumption (3.1) and then applying properties of the geometric series. A similar proof holds for the other three series.

$$\begin{aligned}\left|\frac{2}{n_j}\sum_{i=1}^{n_j-1}\sum_{k=i+1}^{n_j}\Big[P(e_i<0,\,e_k<0)-P(e_i<0)\,P(e_k<0)\Big]\right| &\leq \\ &\leq \frac{2}{n_j}\sum_{i=1}^{n_j-1}\sum_{k=i+1}^{n_j}\Big|P(e_i<0,\,e_k<0)-P(e_i<0)\,P(e_k<0)\Big| \\ &\leq K\frac{2}{n_j}\sum_{i=1}^{n_j-1}\sum_{k=i+1}^{n_j}\rho^{k-i} \\ &= 2K\frac{\rho}{1-\rho}\,\frac{n_j-1}{n_j}-\left[\frac{1}{n_j}\,\frac{\rho^2}{1-\rho^2}\left(1-\rho^{n_j-1}\right)\right] \\ &\leq 2K\frac{\rho}{1-\rho}\,,\end{aligned}$$

where the constants $K>0$ and $0\leq\rho<1$ are given in expression (3.1). The last line follows because the term in brackets is nonnegative and the entire expression is nonnegative. Thus the above series is convergent. Since the other three series follow similarly and, since absolute convergence implies convergence, the series for the variance $\sigma^2_{n_j}$ converges. Let $\sigma^2(0)$ denote the value to which the series converges. The actual value is not needed in the proof but can be obtained from Wendler [20] as noted below.

The fourth condition requires that for all b, $\mathrm{Var}_0\Big\{\sqrt{n_j}\,\big[\overline{S}(b/\sqrt{n_j})-\overline{S}(0)\big]\Big\}\to 0$, as $n_j\to\infty$, where $I(x)=1$ if x is true, 0 otherwise. Based on the sign function, we have

$$V_{n_j,b}\;=_{\text{dfn}}\;\mathrm{Var}\Big[\sqrt{n_j}\,\big[\overline{S}(b/\sqrt{n_j})-\overline{S}(0)\big]\Big]\;=\;\mathrm{Var}\left[\frac{-2}{\sqrt{n_j}}\sum_{i=1}^{n_j}I\big(0<e_i<b/\sqrt{n_j}\big)\right].$$

Thus,

$$\begin{aligned}V_{n_j,b} &= \frac{4}{n_j}\sum_{i=1}^{n_j}\mathrm{Var}\Big[I\big(0<e_i<b/\sqrt{n_j}\big)\Big] \\ &\quad+\frac{8}{n_j}\sum_{i=1}^{n_j-1}\sum_{k=i+1}^{n_j}\mathrm{cov}\Big[I\big(0<e_i<b/\sqrt{n_j}\big),\,I\big(0<e_k<b/\sqrt{n_j}\big)\Big].\end{aligned}\tag{A.2}$$

By stationarity and continuity of the cdf $F(t)$, $E\big[I\big(0<e_i<b/\sqrt{n_j}\big)\big]=F\big(b/\sqrt{n_j}\big)-\frac{1}{2}\to 0$, as $n_j\to\infty$; hence, the variance term on the right side of (A.2) goes to 0 as $n_j\to\infty$.

We can write the covariances as

$$\begin{aligned}c_{n_j,i,k}\;&=_{\text{dfn}}\;\mathrm{cov}\Big[I\big(0<e_i<b/\sqrt{n_j}\big),\,I\big(0<e_k<b/\sqrt{n_j}\big)\Big] \\ &=\;P\Big[0<e_i<b/\sqrt{n_j}\,,\;0<e_k<b/\sqrt{n_j}\Big] \\ &\quad-P\Big[0<e_i<b/\sqrt{n_j}\Big]\,P\Big[0<e_k<b/\sqrt{n_j}\Big].\end{aligned}$$

Notice that this is similar to the above argument on the variance, except that the terms also go to zero as $n_j\to\infty$. Using mean value theorems it follows that the rate of this convergence is $1/n_j$. Using the assumptions from Section 3 and this rate we have $|c_{n_j,i,k}|\leq K\rho_{n_j}^{k-i}$, where $\rho_{n_j}=O(1/n_j)$. Following the same argument as used for the variance, the covariance term in (A.2) in absolute value is less than or equal to

$$2K\frac{\rho_{n_j}}{1-\rho_{n_j}}\leq O(1/n_j)\to 0\,,\qquad \text{as}\quad n_j\to\infty\,.$$

Thus $V_{n_j,b} \to 0$ as $n_j \to \infty$.

By these four conditions, as shown in Chapter 1 of Hettmansperger and McKean [7], the sign process satisfies the linearity result:

$$\sqrt{n_j}\,\overline{S}_j(\theta) \;=\; \sqrt{n_j}\,\overline{S}_j(0) - 2f(0)\sqrt{n_j}\,\theta + o_p(1)\,, \tag{A.3}$$

for $\sqrt{n_j}\,|\theta| \le B$, for all $B > 0$.

To obtain $\sigma^2(0)$, we can use Wendler [20]. He showed, under the mixing conditions above, that $\sqrt{n_j}\,|\hat{\theta}_e|$ converges in distribution and, hence, is tight. Since $\overline{S}_j(\theta) = 0$, we can use (A.3) and Wendler's asymptotic distribution to obtain the asymptotic normal distribution of $\sqrt{n_j}\,\overline{S}_j(0)$.

For our proof, we are interested in the residual process. Since for the proof the true parameters are 0, we can write the residuals as $\hat{e}_i = e_i - \mathbf{x}_i'\hat{\boldsymbol{\beta}}_{LS}$, $i = 1, ..., n_j$. The residual sign process is then given by

$$\overline{S}_j^*(\theta) = \frac{1}{n_j}\sum_{i=1}^{n_j} \operatorname{sgn}(\hat{e}_i - \theta)\,. \tag{A.4}$$

Let $\hat{\theta}^*$ denote median of the residuals. Notice that it solves $\overline{S}_j^*(\hat{\theta}^*) = 0$. In the independent error case, Hettmansperger and McKean [7] established the linearity of the residual process for any root-n consistent estimate of $\boldsymbol{\beta}$; see their Section 3.5 and the associated parts of the Appendix. A key result used in their proof was the linearity for the single sample case, i.e., in the current proof, the result (A.3). See Lemma A.3.2 of Hettmansperger and McKean [7]. The remainder of the proof for the linearity of $\overline{S}_j^*(\theta)$ follows using similar reasoning as above. The result is

$$\sqrt{n_j}\,\overline{S}_j^*(\theta) \;=\; \sqrt{n_j}\,\overline{S}_j^*(0) - 2f(0)\sqrt{n_j}\,\theta + o_p(1)\,, \tag{A.5}$$

for $\sqrt{n_j}\,|\theta| \le B$, for all $B > 0$. Using this and $\overline{S}_j^*(\hat{\theta}^*) = 0$, we obtain the asymptotic distribution of $\hat{\theta}^*$ and, hence, its consistency.

The second part of our proof requires the consistency of three other estimators. The first is the median of the absolute value of the residuals. This is easily obtained by replacing e_i with $|e_i|$ in the above processes. Since the pdf of $|e_i|$ is strictly positive at the true median, the proof holds in this case too. The second estimator is a function of the residuals from two bins, say, j and j'. More specifically, it is a function of the residuals

$$\hat{e}_{j,i} + \hat{e}_{j',i'} \;=\; e_{j,i} + e_{j',i'} - \begin{bmatrix} \mathbf{x}_{j,i}^{\mathsf{T}} & \mathbf{x}_{j',i'}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}}_j \\ \hat{\boldsymbol{\beta}}_{j'} \end{bmatrix},$$

where $\hat{\boldsymbol{\beta}}_j$ and $\hat{\boldsymbol{\beta}}_{j'}$ denote the LS estimates from bins j and j', respectively. Because the vector $(\hat{\boldsymbol{\beta}}_j^{\mathsf{T}}, \hat{\boldsymbol{\beta}}_{j'}^{\mathsf{T}})^{\mathsf{T}}$ is root-n consistent and the convolution of identical pdfs is positive at its median when each pdf is positive at its median, nothing in the above proof precludes the use of random errors of the form $e_{j,i} + e_{j',i'}$. Thus the theory holds in this case also. These comments apply to the third estimator also because it is based on the residuals $\hat{e}_{j,i} - \hat{e}_{j',i'}$.

Part 2 of the Proof:

This part of the proof makes use of the standard inequality $|a| = |a-b+b| \leq |a-b| + |b|$. It suffices to show consistency of $\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}$ element-wise. We first show the consistency of the diagonal elements. The statistic and functional of the m^{th} diagonal of $\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}$ are given by:

$$\mathrm{MAD}\{\hat{\mathbf{e}}_m\} = \mathrm{med}_i\big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| \quad \text{with functional} \quad \xi_m = \mathrm{med}\big|\mathbf{e}_m - \mathrm{med}\{\mathbf{e}_m\}\big|\,.$$

Without loss of generality, assume that $\mathrm{med}\{\mathbf{e}_m\} = 0$. From Part 1, $\mathrm{med}_i\{\hat{\mathbf{e}}_{m_i}\} \xrightarrow{P} 0$, in probability. Next, assume that $\mathrm{med}\{|\mathbf{e}_m|\} = \xi$. Then also from Part 1, $\mathrm{med}_i|\hat{\mathbf{e}}_{m_i}| \xrightarrow{P} \xi$. Choose N_0 sufficiently large so that, given $\varepsilon > 0$,

$$k \geq N_0 \implies \big|\mathrm{med}_{1\leq i \leq k}\{\hat{\mathbf{e}}_{m_i}\}\big| < \varepsilon \tag{A.6}$$

with probability greater than $(1-(\varepsilon/2))$. Let A_n denote the event where (A.6) occurs. Then, on A_n we have

$$\begin{aligned} |\hat{\mathbf{e}}_{m_i}| &= \big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\} + \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| \\ &\leq \big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| + \big|\mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| \\ &< \big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| + \varepsilon\,. \end{aligned}$$

So, on A_n,

$$\mathrm{med}_i|\hat{\mathbf{e}}_{m_i}| < \mathrm{med}_i\big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| + \varepsilon\,, \tag{A.7}$$

and

$$\begin{aligned} \big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| &= \big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\} - \hat{\mathbf{e}}_{m_i} + \hat{\mathbf{e}}_{m_i}\big| \\ &\leq \big|\mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| + |\hat{\mathbf{e}}_{m_i}| \\ &< |\hat{\mathbf{e}}_{m_i}| + \varepsilon\,. \end{aligned}$$

Hence, on A_n,

$$\mathrm{med}_i\big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| < \mathrm{med}_i|\hat{\mathbf{e}}_{m_j}| + \varepsilon\,. \tag{A.8}$$

Putting (A.7) and (A.8) together, we have on A_n,

$$\Big|\mathrm{med}_i\big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| - \mathrm{med}_i|\hat{\mathbf{e}}_{m_i}|\Big| < \varepsilon\,. \tag{A.9}$$

Since this occurs with probability of at least $(1-(\varepsilon/2))$, the difference on the left-side goes to 0 in probability. As noted above, from Part 1, $\mathrm{med}_i|\hat{\mathbf{e}}_{m_i}| \xrightarrow{P} \xi$; hence, $\mathrm{med}_i\big|\hat{\mathbf{e}}_{m_i} - \mathrm{med}_j\{\hat{\mathbf{e}}_{m_j}\}\big| \xrightarrow{P} \xi$.

For the off-diagonal elements, let $m \neq m'$ be given. Recall that the off-diagonal elements of $\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}$ are given by equation (2.2), which can be expressed as follows:

$$\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}(m,m') = \left(\mathrm{MAD}\left\{\frac{\hat{\mathbf{e}}_m \oplus \hat{\mathbf{e}}_{m'}}{2}\right\}\right)^2 - \left(\mathrm{MAD}\left\{\frac{\hat{\mathbf{e}}_m \ominus \hat{\mathbf{e}}_{m'}}{2}\right\}\right)^2. \tag{A.10}$$

It suffices to show consistency for each of the terms on the right-side. Define $\mathbf{t} = \frac{1}{2}\left(\mathbf{e}_m \oplus \mathbf{e}_{m'}\right)$. Then the statistic and its functional, respectively, for the off-diagonal elements are:

$$\mathrm{MAD}\{\hat{\mathbf{t}}\} = \mathrm{med}_i\big|\hat{\mathbf{t}}_i - \mathrm{med}_j\{\hat{\mathbf{t}}_j\}\big| \quad \text{with functional} \quad \xi_{m,m'} = \mathrm{med}\big|\mathbf{t} - \mathrm{med}\{\mathbf{t}\}\big|\,.$$

Without loss of generality let $\mathrm{med}\{\mathbf{t}\} = 0$. From Part 1, $\mathrm{med}_i\{\hat{\mathbf{t}}_i\} \xrightarrow{P} 0$. Then the proof follows in the same manner as for the diagonal elements. So each of the MADs in equation (A.10) is consistent. Therefore, the entire expression is consistent. Thus, the diagonal and off-diagonal entries of $\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}$ are consistent. Hence, $\hat{\mathbf{\Sigma}}_M^{(\mathrm{rob})}$ is a consistent estimator of $\mathbf{\Sigma}_M$. □

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The methods described in this manuscript have been implemented in the `R` programming language. The code is available at https://github.com/jelsema/RRSM. Should the link deprecate, contact the first author for information regarding how to obtain the code.

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ESTIMATION OF SMALL AREA TOTAL WITH RANDOMIZED DATA

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Abstract:

- In social surveys involving questions that are sensitive or personal in nature, respondents may not provide correct answers to certain questions asked by the interviewer. The impact of this non-response or inaccurate response becomes even more acute in the case of small area estimation (SAE) where we already have the problem of small sample size coming from the small area. To obtain a truthful response, we use randomized response techniques in each small area. We assume that a non-sensitive auxiliary variable, highly correlated with the study variable, is available. We use the word model in two senses — one in the context of population models, i.e. the relationship between the study variable and the auxiliary variable; and second, the scrambled response model. We focus on the problem of estimating small area total and examine its performance both theoretically and numerically.

Key-Words:

- *quantitative sensitive variable; randomized response models; small area estimation; superpopulation model.*

1. INTRODUCTION

In social sciences, responses on some stigmatizing variables are often needed to make inference about the behavior of some human populations. Examples of such situations are where questions are asked that are related to topics like tax evasion, use of illegal drugs, extra marital affairs, ethical issues, political affiliation, etc. In the case of stigmatizing study variables, non-sampling error may increase due to missing or false responses, which leads to biased estimates of population parameters such as mean, total or proportion. To reduce such bias in sample surveys, [34] proposed a randomized response technique (RRT) for obtaining more accurate estimates. A lot of research has been done for improving the original RRT model of [34]. Authors contributing in this area include [17], [18], [35], [6], [12], [22], [7], [3], [19, 20], [21] and [9, 10, 11]. In RRT literature, much more attention has been paid to design-based approach which assumes the population to consist of fixed constants. But in many real-life situations, population values are generated as realizations of a set of stochastic variables. Such population is called a superpopulation and the statistical models for such type of populations are called superpopulation models. Superpopulation models help in sample selection, constructing estimators for population parameters of interest, and enhancing the precision of estimates. A superpopulation model uses the relationship between the study variable and the auxiliary variable(s) to predict the population values for the non-sampled units assuming non-informative sampling approach. Under the framework of model-based inference, [14] dealt with the problem of estimation of a finite population mean or total. [27] and [8] attempted to obtain optimal model-unbiased estimators of the population mean and total using least squares estimation methods and the well-known Gauss–Markov theorem. Some discussion on model-based approach can be found in [2], [15], [16], [30, 31], [29], [28], and [33]. A detailed review of model-based estimation is also available in [32].

[13] and [24] have suggested post-censal estimates (estimates obtained immediately after census using the census results) for small areas and called it small area estimation (SAE). [23] dealt with labor force trend estimation for small areas. Work related to such methods can also be found in [25, 26] and [38]. More recently, [36] have considered estimation of uncertainty in spatial micro-simulation approaches for SAE. The main purpose of SAE is to overcome the problem of small sample when separate estimates for domains are needed. In this article, we develop some model-based estimators for small area totals assuming the study variable in each domain is sensitive. A generalized randomized response model has been used to collect information about the study variable. The rest of the article is structured as follows: an overview of SAE under direct response is considered in Section 2 with some superpopulation models. Section 3 extends the SAE given in Section 2 to randomized response models, assuming a sensitive quantitative study variable and non-sensitive auxiliary variable. Section 4 presents a numerical study based on two real life data sets. Some concluding remarks are provided in Section 5.

2. SAE UNDER DIRECT RESPONSE

Consider a finite population $U = \{U_1, U_2, ..., U_N\}$ of N units as a realization of a superpopulation with variable of interest y, and auxiliary variable x. For a specific sup-population A_k, also known as "small area", let d_{ki} be an area specific binary variable, for $k = 1, 2, 3, ...m$ and $i = 1, 2, ...N$, such that $d_{ki} = 1$ if U_i belongs to A_k, and zero otherwise. Further, let $N_k = \sum_U d_{ki}$ be the size of the k-th sub-population or k-th small area (usually unknown), $T_{yk} = \sum_U d_{ki}\, y_i$ and $T_{xk} = \sum_U d_{ki}\, x_i$ be the population totals, $\mu_{yk} = \frac{T_{yk}}{N_k}$ and $\mu_{xk} = \frac{T_{xk}}{N_k}$ be the population means, and $\sigma^2_{yk} = \frac{1}{N_k} \sum_U d_{ki}(y_i - \mu_{yk})^2$ and $\sigma^2_{xk} = \frac{1}{N_k} \sum_U d_{ki}(x_i - \mu_{xk})^2$ be the population variances of the study variable and the auxiliary variable respectively in the k-th area. The notation $\sum_U$ is used for summing the values over U. Also, let the covariance between the study variable and the auxiliary variable in the k-th area be $\sigma_{yxk} = \frac{1}{N_k} \sum_U d_{ik}\,(y_i - \mu_{yk})\,(x_i - \mu_{xk})$. Suppose that s is a member of the set S of all possible samples that can be drawn from U using simple random sampling without replacement (SRSWOR) scheme with size n, and $\bar{s}$ consists of all those elements of U that are not selected in sample s. The population total for the study variable, quantity of interest or estimand, in k-th area can then be expressed as $T_{yk} = \sum_s d_{ki}\, y_i + \sum_{\bar{s}} d_{ki}\, y_i$. A predictor for T_{yk} is obtained as follows:

$$\hat{T}_{yk} = \sum_s d_{ki}\, y_i + \sum_{\bar{s}} d_{ki}\, \hat{y}_i\,. \tag{2.1}$$

The main problem is to find $\hat{y}_i$ for $U_i \in \bar{s}$. The predictor $\hat{y}_i$ is obtained assuming different superpopulation models. We consider three most widely used population models:

1. Homogenous Population Model (HPM): $y = \mu_{yk} + \varepsilon\,,$
2. Linear Population Model (LPM): $y = \alpha_k + \beta x + \varepsilon\,,$
3. Ratio Population Model (RPM): $y = \gamma x + x^{1/2} \varepsilon\,,$

for $k = 1, 2, ..., m$, where ε is the stochastic error term which has mean 0 and a constant variance σ^2. Also, μ_{yk} and α_k are mean effects in k-th area and β and γ are the coefficients of the regression line of y on x for the whole population for the cases with and without intercepts. In model based approach, these parameters are termed as superpopulation parameters.

2.1. Homogeneous Population Model (HPM)

In case of HPM, a BLUP for μ_{yk}, obtained by minimizing the residual sum of square $\sum_s d_{ki}(y_i - \mu_{yk})^2$ is $\bar{y}_k = \frac{1}{n_k} \sum_s d_{ki}\, y_i$, which yields an estimator for T_{yk} given by

$$\hat{t}_{k\text{h}} = \sum_s d_{ki}\, y_i + \sum_{\bar{s}} d_{ki}\, \bar{y}_k = \frac{N}{n} \sum_s d_{ki}\, y_i\,. \tag{2.2}$$

The sub-script 'h' is used to indicate that the superpopulation model is homogeneous. It is straight forward to show that $\hat{t}_{k\text{h}}$ is an unbiased estimator of population total T_{yk} with variance given by

$$\text{Var}(\hat{t}_{k\text{h}}) = \lambda\big[\theta_k\, \sigma^2_{yk} + \theta_k(1 - \theta_k)\, \mu^2_{yk}\big]\,, \tag{2.3}$$

where $\theta_k = \frac{N_k}{N}$ is the population proportion of the units belonging to k-th small area, and $\lambda = \frac{N(N-N)}{n}$. For proof readers can see [5, p. 156–160].

2.2. Linear Population Model (LPM)

Now consider LPM for finding $\hat{y}_i$, $U_i \in \bar{s}$. The BLUP for α_k and β are obtained by minimizing the sum of squared prediction errors for specific areas, i.e.

$$\text{SSPE} = \sum_s d_{ki}(y_i - \alpha_k - x_i\beta)^2 .$$

These are given by $\hat{\alpha}_k = \bar{y}_k - \hat{\beta}\bar{x}_k$ and $\hat{\beta} = \frac{\sum_s d_{ki}(y_i-\bar{y}_k)(x_i-\bar{x}_k)}{\sum_s d_{ki}(x_i-\bar{x}_k)^2}$, where $\bar{y}_k$ and $\bar{x}_k$ are the sample means corresponding to k-th small area. The estimator of T_{yk} under LPM is given by

$$\hat{t}_{k\text{lr}} = \sum_s d_{ki}\, y_i + \sum_{\bar{s}} d_{ki}\big(\hat{\alpha}_k + \hat{\beta} x_i\big) .$$

After some simplifications and using assumption from [5], i.e. $\frac{N_k}{N} \approx \frac{n_k}{n}$, we get

$$\hat{t}_{k\text{lr}} = \frac{N}{n} t_{yk} + \hat{\beta}\bigg(T_{xk} - \frac{N}{n} t_{xk}\bigg), \tag{2.4}$$

where $t_{yk} = \sum_s d_{ki}\, y_i$ and $t_{xk} = \sum_s d_{ki}\, x_i$ are the sample totals for k-th small area. Further, $\hat{\beta}$ given in (2.4) is based on local (area specific) observations only, which do not account for relationship between the variables for the entire population. To overcome this deficiency, different area level models have been proposed in literature. For simplicity, we assume that the regression coefficient β of y on x is known for the whole population. For known β, we have

$$\hat{t}_{k\text{lr}} = \frac{N}{n} t_{yk} + \beta\bigg(T_{xk} - \frac{N}{n} t_{xk}\bigg). \tag{2.5}$$

The sub-script ‘lr’ is used to denote that the underlying model is linear. For known β, $\hat{t}_{k\text{lr}}$ is unbiased for T_{yk} with variance given by

$$\text{Var}(\hat{t}_{k\text{lr}}) = \lambda\big(\sigma^{*2}_{yk} + \beta^2 \sigma^{*2}_{xk} - 2\beta\, \sigma^*_{yxk}\big) , \tag{2.6}$$

where $\sigma^{*2}_{yk} = \theta_k \sigma^2_{yk} + \theta_k(1-\theta_k)\mu^2_{yk}$, $\sigma^{*2}_{xk} = \theta_k \sigma^2_{xk} + \theta_k(1-\theta_k)\mu^2_{xk}$ and $\sigma^*_{yxk} = \theta_k \sigma_{yxk} + \theta_k(1-\theta_k)\,\mu_{yk}\,\mu_{xk}$. The value of β that minimizes the variance is $\beta_{\text{opt}} = \frac{\sigma^*_{yxk}}{\sigma^{*2}_{xk}}$. The corresponding minimum variance of $\hat{t}_{k\text{lr}}$ is given by

$$\text{Var}(\hat{t}_{k\text{lr}})_{\text{opt}} = \lambda\,\big(1 - \rho^{*2}_{yxk}\big)\,\sigma^{*2}_{yk} , \tag{2.7}$$

where $\rho^*_{yxk} = \frac{\sigma^*_{yxk}}{\sigma^*_{yk}\sigma^*_{xk}}$. From Equations (2.7) and (2.3), it is obvious that $\hat{t}_{k\text{lr}}$ is always more efficient than $\hat{t}_{k\text{h}}$ for any linear relationship between y and x.

2.3. Ratio Population Model (RPM)

For situations when there is a proportional relationship between the survey variable and the auxiliary variables, the RPM [32] is often preferred as the working model. RPM is given by

$$y = \gamma x + x^{1/2}\varepsilon \,. \tag{2.8}$$

The estimator for γ which minimizes the sum of squared errors, i.e. $\text{SSE}^* = \sum_s d_{ki}\big(\frac{y_i - x_i\gamma}{x_i^{1/2}}\big)^2$, is given by $\hat{\gamma} = \frac{\sum_s d_{ki}\, y_i}{\sum_s d_{ki}\, x_i}$. Now consider

$$\hat{t}_{k\mathrm{r}} = \sum_s d_{ki}\, y_i + \sum_{\bar{s}} d_{ki}(\hat{\gamma} x_i) \tag{2.9}$$

as an estimator of T_{yk}. The sub-script 'r' is used to denote the ratio population model for the response variable. After simplification and assuming $\frac{N_k}{N} \approx \frac{n_k}{n}$, we get

$$\hat{t}_{k\mathrm{r}} \;=\; \frac{\sum_s d_{ki}\, y_i}{\sum_s d_{ki}\, x_i} \sum_{\bar{s}} d_{ki}\, x_i \;=\; \frac{N}{n}\left[t_{yk}\,\frac{n\,\mu_{xk}}{t_{xk}}\right]. \tag{2.10}$$

The bias and MSE respectively, of $\hat{t}_{k\mathrm{r}}$, are given by

$$\text{Bias}(\hat{t}_{k\mathrm{lr}}) \cong \frac{\lambda}{N}\,\mu_{yk}\big(C_{xk}^{*2} - C_{yxk}^{*}\big) \tag{2.11}$$

and

$$\text{MSE}(\hat{t}_{k\mathrm{r}}) \cong \lambda\mu_{yk}^2\big(C_{yk}^{*2} + C_{xk}^{*2} - 2\,C_{yxk}^{*}\big)\,, \tag{2.12}$$

where $C_{yk}^{*2}{=}\frac{\sigma_{yk}^{*2}}{\mu_{yk}^2}$, $C_{xk}^{*}{=}\frac{\sigma_{xk}^{*2}}{\mu_{xk}^2}$ and $C_{yxk}^{*}{=}\frac{\sigma_{yxk}^{*}}{\mu_{yk}\,\mu_{yk}}$. From (2.3) and (2.12), it can be inferred that $\text{MSE}(\hat{t}_{k\mathrm{r}}) \leq \text{Var}(\hat{t}_{k\mathrm{h}})$ if $\rho_{yxk}^{*} \geq \frac{1}{2}\,\frac{C_{xk}^{*}}{C_{yk}^{*}}$.

3. SAE UNDER RANDOMIZED RESPONSE TECHNIQUE

When the study variable is of sensitive nature, it is difficult to obtain 100% response through direct response method. For improved response rate in such situations, survey statisticians prefer to use RRT. Assuming quantitative study variable, and following [11], we use the following scrambled response model

$$z = a\,y + b\,, \tag{3.1}$$

where y is the sensitive study variable which follows one of the population models given in Section 2, a and b are two uncorrelated scrambling variables with means μ_a and μ_b, and variances σ_a^2 and σ_b^2 respectively. Further, a and b are independent of the study variable y. Note that respondents from each small area use the same scrambling variables a and b whose distributions are unknown to the interviewer while the means and variances are known. Taking expectation of Equation (3.1) with respect to randomization mechanism, we have $E_R(z) = \mu_a\, y + \mu_b$. The transformed scrambled response is obtained as $y = \frac{E_R(z) - \mu_b}{\mu_a}$. A sample unbiased estimate for y is $\tilde{y} = \frac{z - \mu_b}{\mu_a}$.

3.1. Homogeneous Population Model (HPM)

When the underlying population model is homogeneous, i.e. when there is no covariate affecting the outcome variable, a BLUP for the superpopulation parameter μ_{yk} is $\tilde{\bar{y}}_k = \tilde{t}_{yk}/n_k$ which yields an estimator for T_{yk} given by

$$\tilde{t}_{k\mathrm{h}} \;=\; \sum_s d_{ki}\,\tilde{y}_i + \sum_{\bar{s}} d_{ki}\,\tilde{\bar{y}}_k \;=\; n_k\,\tilde{\bar{y}}_k + (N_k - n_k)\,\tilde{\bar{y}}_k \;=\; \frac{N}{n}\,\tilde{t}_{yk}\,, \tag{3.2}$$

where $\tilde{t}_{yk} = \sum_s d_{ki}\,\tilde{y}_i$. We assume that the sampling weights for the whole sample and the sample within k-th domain are same, i.e. $\frac{N_k}{N} \approx \frac{n_k}{n}$. It is easy to show that $\tilde{t}_{k\mathrm{h}}$ is an unbiased estimator of population total T_{yk} with variance

$$\mathrm{Var}(\tilde{t}_{k\mathrm{h}}) \;=\; \lambda\big(\theta_k\,\tilde{\sigma}^2_{yk} + \theta_k(1-\theta_k)\,\mu^2_{yk}\big)\,, \tag{3.3}$$

where $\tilde{\sigma}^2_{yk} = \mathrm{Var}(\tilde{y}_i \,|\, d_{ki}\!=\!1) = \frac{1}{\mu_a^2}\,\mathrm{Var}(z_i \,|\, d_{ki}\!=\!1)$, and

$$\begin{aligned}\mathrm{Var}(z_i \,|\, d_{ki}\!=\!1) \;&=\; V_s\big\{E_R(z_i \,|\, d_{ki}\!=\!1)\big\} + V_R\big\{E_S(z_i \,|\, d_{ki}\!=\!1)\big\}\\ &=\; E_s\big(\sigma_a^2\,y_i^2 + \sigma_b^2 \,|\, d_{ki}\!=\!1\big) + V_s\big(\mu_a\,y_i + \mu_b \,|\, d_{ki}\!=\!1\big)\\ &=\; \sigma_a^2\,\mu_{2,yk} + \sigma_b^2 + \mu_a^2\,\sigma^2_{yk}\,,\end{aligned} \tag{3.4}$$

where E_s and V_s are the expectation and variance with respect to the data generating mechanism. Also $\mu_{2,yk}$ is the second order raw moment for k-th area. Using value of $\tilde{\sigma}^2_{yk}$ from (3.3), we get

$$\begin{aligned}\mathrm{Var}(\tilde{t}_{k\mathrm{h}}) \;&=\; \lambda\big(\theta_k\,\sigma^2_{yk} + \theta_k(1-\theta_k)\,\mu^2_{yk} + \theta_k\,\psi^2_{yk}\big)\,,\\ \mathrm{Var}(\tilde{t}_{k\mathrm{h}}) \;&=\; \mathrm{Var}(\hat{t}_{k\mathrm{h}}) + \lambda\big(\theta_k\,\psi^2_{yk}\big)\,,\end{aligned} \tag{3.5}$$

where $\psi^2_{yk} = \frac{1}{\mu_a^2}\,\big(\sigma_a^2\,\mu_{2,yk} + \sigma_b^2\big)$. It is observed from (3.5) that $\mathrm{Var}(\tilde{t}_{k\mathrm{h}})$ is always larger than $\mathrm{Var}(\hat{t}_{k\mathrm{h}})$ as the second term is positive. For detailed derivation, see [1]. The $\mathrm{Var}(\tilde{t}_{k\mathrm{h}})$ decreases with decrease in variance of the scrambled variables but this leads to reduction in respondent's privacy as well. Hence, the variance of the scrambled response models should be of a reasonable size resulting in a proper tradeoff between respondent's privacy and the efficiency of the proposed estimators.

To improve efficiency for a fixed level of privacy protection, we use model relationship between the available auxiliary variable and the study variable. Subsections 3.2 and 3.3 cover linear and ratio population models respectively that utilize the relationship between the variables at unit level to increase efficiency.

3.2. Linear Population Model (LPM)

Assuming LPM, we find the predicted transformed scrambled response $\tilde{y}_i$, $U_i \in \bar{s}$. The BLUP for α_k and β are obtained by minimizing the sum of squared errors for the k-th area as follows:

$$\mathrm{SSE} \;=\; \sum_s d_{ki}\,\tilde{e}_i^2 \;=\; \sum_s d_{ki}(\tilde{y}_i - \alpha_k - x_i\beta)^2\,,$$

where $\tilde{\hat{\alpha}}_k = \tilde{\bar{y}}_k - \tilde{\hat{\beta}}\,\bar{x}_k$ and $\tilde{\hat{\beta}} = \frac{\sum_s d_{ki}(\tilde{y}_i - \tilde{\bar{y}}_k)\,(x_i - \bar{x}_k)}{\sum_s d_{ki}(x_i - \bar{x}_k)^2}$. The predictive estimator under LPM using transformed scrambled response is given by

$$\tilde{t}_{k\mathrm{lr}} \;=\; \sum_s d_{ki}\,\tilde{y}_i + \sum_{\bar{s}} d_{ki}\big(\tilde{\hat{\alpha}}_k + \tilde{\hat{\beta}}\,x_i\big)\,. \tag{3.6}$$

After some simplification, we get

$$\tilde{t}_{k\mathrm{lr}} \;=\; \frac{N}{n}\,\tilde{t}_{yk} + \tilde{\hat{\beta}}\left(T_{xk} - \frac{N}{n}\,t_{xk}\right).$$

By same argument as given in Subsection 2.2, we have

$$\tilde{t}_{k\mathrm{lr}} \;=\; \frac{N}{n}\,\tilde{t}_{yk} + \beta\left(T_{xk} - \frac{N}{n}\,t_{xk}\right). \tag{3.7}$$

For known β, $\tilde{t}_{k\mathrm{lr}}$ is unbiased for T_{yk}, with variance given by

$$\operatorname{Var}(\tilde{t}_{k\mathrm{lr}}) \;=\; \lambda\left(\tilde{\sigma}^{*2}_{yk} + \beta^2\,\sigma^{*2}_{xk} - 2\,\beta\,\sigma^*_{yxk}\right). \tag{3.8}$$

The optimum value of β is $\beta_{\mathrm{opt}} = \frac{\sigma^*_{yxk}}{\sigma^{*2}_{xk}}$ with corresponding design optimum variance

$$\operatorname{Var}(\tilde{t}_{k\mathrm{lr}})_{\mathrm{opt}} \;=\; \lambda\left(1 - \tilde{\rho}^{*2}_{yxk}\right)\tilde{\sigma}^{*2}_{yk}\,, \tag{3.9}$$

where $\tilde{\rho}^*_{yxk} = \frac{\sigma^*_{yxk}}{\tilde{\sigma}^*_{yk}\,\sigma^*_{xk}}$. Equation (3.9) shows that $\tilde{t}_{k\mathrm{lr}}$ is always more efficient than $\tilde{t}_{k\mathrm{h}}$ for any correlation between y and x.

3.3. Ratio Population Model (RPM)

For the situation when there is a proportional relationship between the sensitive study variable, and the auxiliary variable whose values are available for all population units and the variance of the survey variable is also proportional to the auxiliary variable, the RPM is often preferred. Consider (3.1), where y follows the ratio population model. The estimator for γ which minimizes the sum of squared errors, i.e. $\mathrm{SSE}^* = \sum_s d_{ki}\big(\frac{\tilde{y}_i - x_i\gamma}{x_i^{1/2}}\big)^2$, is given by $\tilde{\hat{\gamma}} = \frac{\sum_s d_{ki}\,\tilde{y}_i}{\sum_s d_{ki}\,x_i}$. Consider the prediction problem as follows

$$\tilde{t}_{k\mathrm{r}} \;=\; \sum_s \tilde{d}_{ki}\,\tilde{y}_i + \sum_{\bar{s}} d_{ki}\big(\tilde{\hat{\gamma}}\,x_i\big)\,. \tag{3.10}$$

After simplification, we get

$$\tilde{t}_{k\mathrm{r}} \;=\; \frac{\sum_s d_{ki}\,\tilde{y}_i}{\sum_s d_{ki}\,x_i}\sum_{\bar{s}} d_{ki}\,x_i \;=\; \frac{N}{n}\left[\tilde{t}_{yk}\,\frac{n\,\mu_{xk}}{t_{xk}}\right]. \tag{3.11}$$

The bias and MSE of $\tilde{t}_{k\mathrm{r}}$ are given by

$$\operatorname{Bias}(\tilde{t}_{k\mathrm{lr}}) \;\cong\; \frac{\lambda}{N}\,\mu_{yk}\big(C^{*2}_{xk} - C^*_{yxk}\big) \tag{3.12}$$

and

$$\operatorname{MSE}(\tilde{t}_{k\mathrm{r}}) \;\cong\; \lambda\mu^2_{yk}\big(\tilde{C}^*_{yk} + \tilde{C}^*_{xk} - 2\,C^*_{yxk}\big)\,, \tag{3.13}$$

where $\tilde{C}^{*2}_{yk} = \frac{\tilde{\sigma}^{*2}_{yk}}{\mu^2_{yk}}$ and $C^*_{yxk} = \frac{\sigma^*_{yxk}}{\mu_{yk}\,\mu_{xk}}$. Equation (3.12) shows that the use of RRT to collect response on the dependent variable does not affect the bias of ratio estimator. From (3.5) and (3.13), it can be inferred that $\operatorname{MSE}(\tilde{t}_{k\mathrm{r}}) \le \operatorname{Var}(\tilde{t}_{k\mathrm{h}})$ if $\tilde{\rho}^*_{yxk} \ge \frac{1}{2}\,\frac{C^*_{xk}}{\tilde{C}^*_{yk}}$.

4. NUMERICAL STUDY

For numerical validation of our proposed estimators, two real life data sets, one with two small areas and the other with three small areas, are used. The detailed descriptions along with summary statistics of the populations are given in following subsections.

Blood transfusion data

The data are taken from [37], where F, the frequency of donations, is the study variable, T (Time in months since first donation) is taken as the covariate, and a binary variable representing whether he/she donated blood in March 2007 (1 stands for donating blood; 0 stands for not donating blood) is taken as the area membership variable.

Players head circumference data

This data is taken from [4] which contains physical measures of $N = 90$ players forming three groups, i.e. high school football players (Group 1), college football players (Group 2) and Non-football players (Group 3), each having 30 students. The three groups represent the small areas. The study variable y and the auxiliary variable x respectively are jaw width and ear-to-top-of-head measurement of players. The scrambling variables a and b are generated from Uniform distributions with different ranges.

Table 1: Summary statistics.

Parameter	**Data 1**		**Data 2**		
k	1	2	1	2	3
θ_k	0.7620	0.2380	0.3333	0.3333	0.3333
μ_{yk}	4.8018	7.7978	13.0833	10.0800	10.9467
μ_{xk}	4.8018	7.7978	14.7333	13.4533	13.6967
σ^2_{yk}	22.5318	64.5916	1.0876	1.1520	1.4577
σ^2_{xk}	605.4251	558.3500	0.8920	0.5702	0.3921
σ_{yxk}	76.3885	140.5756	0.5402	0.0870	0.0870
ρ_{yxk}	0.6540	0.7402	0.3333	0.3333	0.3333

Table 1 provides the summary statistics for the data sets. The theoretical results (TR) are obtained using Variance/MSE expressions given in Section 2. The simulated results (SR) are obtained using following algorithm:

1. Select a simple random sample of size n (100 and 30 for Populations I and II respectively) without replacement from the populations described above and stratify the populations according to the domain membership variable d_k.

2. Record information y and x for all small areas after generating values of scrambling variables a and b from uniform distribution with different ranges.
3. Calculate the values of small area estimators under direct and randomized response technique.
4. Repeat Steps 1–3 50000 times and obtain the simulated Variance, MSE and PRE.

The PRE in Table 2 are computed as $\mathrm{PRE_r} = \frac{\mathrm{Var}(\hat{t}_{k\mathrm{h}})}{\mathrm{MSE}(\hat{t}_{k\mathrm{r}})}$ and $\mathrm{PRE_{lr}} = \frac{\mathrm{Var}(\hat{t}_{k\mathrm{h}})}{\mathrm{Var}(\hat{t}_{k\mathrm{lr}})}$ for $\hat{t}_{k\mathrm{r}}$ and $\tilde{t}_{k\mathrm{lr}}$ are respectively while $\mathrm{PRE_h}$ is 100 for $\hat{t}_{k\mathrm{h}}$. Table 2 gives the theoretical and simulated PREs of the small area total estimators for different domains under direct response (without using randomized response techniques) with both data sets. PREs in Tables 3 and 4 are obtained in similar manner using the Variances and MSEs under RRT. The theoretical and simulated values of PRE are reported in Tables 2–4 with notations TR and SR respectively.

Table 2: PREs of the SAE under direct response.

		Type	$\mathrm{PRE_h}$	$\mathrm{PRE_r}$	$\mathrm{PRE_{lr}}$
Data I	$k = 1$	TR	100	215.864	216.839
		SR	100	217.230	218.106
	$k = 2$	TR	100	378.592	379.123
		SR	100	370.443	375.775
Data II	$k = 1$	TR	100	13853.214	13862.216
		SR	100	12993.771	14382.960
	$k = 2$	TR	100	5134.249	5137.867
		SR	100	4855.831	5352.376
	$k = 3$	TR	100	6770.974	6770.974
		SR	100	6371.760	7076.799

From Table 2, one can infer that for both data sets, total estimators under RPM and LPM (see the last two columns) which utilize auxiliary information provide smaller variance than the MSE of Total estimator under HPM. Further, estimator obtained through LPM outperforms the other two competitors in all cases.

Tables 3 and Table 4 give a comparison of the three competing population models in term of PREs for Data I and Data II respectively under randomized response. Going from top to bottom in Tables 3 and 4, we observe that the PREs decrease with increase in variability in the scrambling variables. Also, comparing Table 2 with Tables 3 and 4, we can infer that the efficiency of the domain estimators decreases when using randomized response technique. But that is expected given that RRT introduces noise in the data. Without RRT, the real loss of efficiency will be much larger due to “invisible” response bias.

Table 3: PRE of the SAE under randomized response for Data I.

	a	b	Type	PRE$_{\text{h}}$	PRE$_{\text{r}}$	PRE$_{\text{lr}}$
$k=1$	$U(2,3)$	$U(0,1)$	TR	100	210.572	211.480
			SR	100	210.726	211.501
		$U(0,5)$	TR	100	208.031	208.907
			SR	100	207.984	208.938
	$U(1,4)$	$U(0,1)$	TR	100	181.451	182.026
			SR	100	179.096	179.553
		$U(0,5)$	TR	100	180.063	180.625
			SR	100	177.685	178.235
$k=2$	$U(2,3)$	$U(0,1)$	TR	100	363.439	363.921
			SR	100	355.997	360.266
		$U(0,5)$	TR	100	360.746	361.220
			SR	100	351.889	357.175
	$U(1,4)$	$U(0,1)$	TR	100	284.007	284.270
			SR	100	275.869	277.921
		$U(0,5)$	TR	100	282.689	282.949
			SR	100	273.902	276.442

Table 4: PRE of the SAE under randomized response for Data II.

	a	b	Type	PRE$_{\text{h}}$	PRE$_{\text{r}}$	PRE$_{\text{lr}}$
$k=1$	$U(2,3)$	$U(0,1)$	TR	100	3740.45	3740.97
			SR	100	2624.11	2797.29
		$U(0,5)$	TR	100	3403.93	3404.35
			SR	100	2368.88	2524.28
	$U(1,4)$	$U(0,1)$	TR	100	631.56	631.57
			SR	100	435.21	460.29
		$U(0,5)$	TR	100	623.77	623.78
			SR	100	429.72	454.59
$k=2$	$U(2,3)$	$U(0,1)$	TR	100	2578.63	2579.54
			SR	100	1991.16	2127.92
		$U(0,5)$	TR	100	2318.17	2318.90
			SR	100	1758.21	1875.70
	$U(1,4)$	$U(0,1)$	TR	100	593.55	593.59
			SR	100	424.67	447.19
		$U(0,5)$	TR	100	582.27	582.31
			SR	100	416.73	438.87
$k=3$	$U(2,3)$	$U(0,1)$	TR	100	2930.02	2930.02
			SR	100	2203.50	2354.74
		$U(0,5)$	TR	100	2642.70	2642.70
			SR	100	1967.09	2095.90
	$U(1,4)$	$U(0,1)$	TR	100	608.22	608.22
			SR	100	432.67	455.85
		$U(0,5)$	TR	100	598.12	598.12
			SR	100	426.19	448.82

5. CONCLUSION

In this study, an attempt for obtaining separate total estimates for the sensitive study variable in each domain (small area) is made using the model relationship between the sensitive study variable and the auxiliary variable. It is observed that the small area total estimators under randomized response techniques possess larger variance (as they should) as compared to the estimators obtained through direct responses. As the privacy and efficiency move in opposite directions, one can't improve both at the same time. Our proposed estimators provide greater efficiency in estimating small area totals when an appropriate model relationship between the study variable and the auxiliary variable is used. Our numerical study with two real life data sets supports the theoretical findings. This is clear from the fact that both $\mathrm{PRE_r}$ and $\mathrm{PRE_{lr}}$ are greater than $\mathrm{PRE_h}$.

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