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Let there be v treatments arranged in b of size k_j each, $j = 1,2, \ldots, b$, with the replication of ith treatment being r_i, $i = 1,2, \ldots, v$. Let $\mathbf{N} = ((n_{ij}))$, where n_{ij} is the replication of ith treatment in jth block. Let $\mathbf{r}' = (r_1, r_2, \cdots, r_v)$. Define N_{ij}^{uv} and $U_{sv}^{(\alpha,\beta)}$ or ST_1. $\mathbf{0}_u$ will denote a column vector of order $u \times 1$ and $\mathbf{1}_s$ would denote a vector of order $s \times 1$. Please note that the multiplication sign throughout the text and in the equations would be as just displayed in the preceding sentence and not as x. Similarly a minus sign, be it in text or in tables or in equations, will be represented as "–" and not as "-"

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Parsad, R., Chandra, H., Mandal, B. N. and Gupta, V. K. (2020).

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Dibley, M. J., Godsby, J. B., Staehling, N. W. and Trowbridge, F. L. (1987). Development of normalized curves for the international growth reference: historical and technical considerations. *American Journal of Clinical Nutrition*, **46(5)**, 736-748.
Datta, G. S., Torabi, M., Rao, J. N. K. and Liu, B. (2018). Small area estimation with multiple covariates measured with errors: A nested error linear regression approach of combining multiple surveys. *Journal of Multivariate Analysis*, **167**, 49-59.

B. Book/ Project/Technical reports

Tiwari, N., Joshi, J. and Upreti, P. K. (2012). *Investigation of Geo-Spatial Hotspots for the Occurrence of Tuberculosis*. Lambert Academic Publishing, Germany (ISBN: 978- 3-8484-0806-1).
Rao, J. N. K. and Molina, I. (2015). *Small Area Estimation*. 2nd Edition, Wiley, Hoboken, NJ.

Csorgo, M., Dawson, D. A., Rao, J. N. K. and Saleh, A. K. Md. E. S. (Eds.) (1981). *Statistics and Related Topics*. North-Holland, Amsterdam.

Binder, D. A., Gratton, M., Hidiroglou, M. A. and Rao, J. N. K. (1984). Analysis of categorical data from surveys with complex designs: some Canadian experiences. In *Proceedings of a Seminar held in Luxemburg*, Eurostat News, Special Number, 75-94.

C. Government Reports

National Institute of Nutrition and Institute of Applied Statistics and Development Studies (2002). *Nutrition Profile of Community in Uttar Pradesh. District Level Reports*. Department of Women and Child Development/Food and Nutrition Board, Government of India.

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1.   Introduction

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A regression model describes the influence of various factors on the response under study. In agricultural experiments, regression models are used to study the effect of manure on the yield of a crop.

2. The Problem and Its Perspectives
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Suppose the manure applied during sowing of the crop is a q-component mixture with mixing proportions given by $\mathbf{x}' = (x_1, x_2, \cdots, x_q)$, where $\mathbf{x} \in \Xi$ $\{(x_1, x_2, \cdots, x_q)|x_i \geq 0, 1 \leq x_i \geq 1, \sum_{i=1}^{q} x_i = 1\}$.

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IN THE SEQUENCE IS GIVEN A TEMPLATE THAT CAN BE USED FOR PREPARATION OF MANUSCRIPT

Estimation and Geo-Spatial Mapping of Incidence of Indebtedness in the State of Karnataka in India by Juxtaposing Survey and Census Data

V.K. Gupta[1], Hukum Chandra[2], Jyotirmoy Sarkar[3], B.N. Mandal[2] and Rajender Parsad[2]

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Abstract

Information about the household debt behaviour in different occupational categories is of key importance to the Governmental organization for taking effective policy measures targeting the vulnerable groups. The purpose of this paper is to illustrates small area estimation (SAE) methodology to estimate extent of indebtedness in rural areas for the two major occupation categories- rural cultivator and rural non-cultivator as well as for both categories combined together across all the 30 districts of Karnataka state in India using the data of All India Debt and Investment Survey 2012-13 and population census 2011. The findings show that the district-level estimates of incidence of indebtedness obtained from SAE are more precise than the direct survey estimates. A spatial map has also been produced to observe the inequality in distribution of indebtedness within districts and in each occupational category across districts. Such maps are definitely useful for framing consistent policy actions and fund disbursement for the indebted household mass.

Key words: Small area estimation; Generalized linear mixed model; Covariates; Principal component analysis; Indebtedness; Spatial Map.

1. Introduction

Agriculture plays an important role in the economy of Karnataka and it is the main occupation for more than 60% of population. Karnataka is a drought-prone region with a large proportion of wasteland and having the second largest arid zone in the country after Rajasthan. And due to these factors, the state has been facing agrarian distress with increasing incidence of farmers' suicides since 1997. In fact, the rate of farmer suicides in Karnataka has hit the highest level in a decade, topping the list after Maharashtra, highlighting agrarian distress in the state, according to the report Accidental Deaths and Suicides in India 2015 published by National Crime Records Bureau (NCRB). According to NCRB 2015 data, about 1,197 farmers committed suicides in Karnataka during 2014-15; the state was just behind Maharashtra and Telangana. The NCRB also found that about 79% suicides (946 out of 1,197) in Karnataka were due to bankruptcy or indebtedness. The pre-requisite for any effective policy approach taken in this regard is a proper statistical and economic framework that allows for an effective

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analysis and monitoring of farmers' distress. Measure of disaggregated level indebtedness can be an important tool to the policy makers to mark certain region or group for upliftment and reduce the situation of agrarian distress or farmers' suicides. In this study we attempt to estimate such micro or disaggregated level incidence of indebtedness at micro or local level using the area level small area model.

Most of the large-scale surveys are planned to produce reliable estimates at macro or higher geographical (*e.g.* national and state) level, and cannot be used directly to generate reliable micro or local (also referred to as small area) level estimates because of the small sample sizes (Rao and Molina 2015). This is because, large scale survey designed for a large population (*e.g.* national and state level) may select a small number of units or even no unit from the small area of interest (*e.g.* district or further disaggregation of district). Hence, sample sizes from small areas (or small domains) are too small to justify the use of traditional direct survey estimates. The underlying theory in the literature of survey sampling that helps in resolving the problem of smaller sample sizes is referred as small area estimation (SAE) technique. The technique is model-based methods that links the variable of interest from survey with the auxiliary information available from other data sources for small areas and hence increase the overall (effective) sample size and precision. In this paper we employ area level SAE technique to produce reliable estimates of the incidence of indebtedness among cultivators and non-cultivators categories as well as for both the categories combined in different districts of rural areas of Karnataka in India by linking data from the All-India Debt and Investment Survey (AIDIS) 2012-13 of National Sample Survey Office (NSSO), and the Population Census 2011. This work will enable us to obtain spatial distribution of incidence of indebtedness as well as regional inequality in such measure of indebtedness among the farm families and other families of rural areas in Karnataka. The rest of the paper has been organized into five sections. In Section 2, we discuss the data used in the paper. Section 3 provides an overview of SAE technique that has been used to generate incidence of indebtedness among occupational category by districts in Karnataka. In Section 4, we present diagnostic procedures to examine model assumptions and validate small area estimates including discussion about the results. Finally, Section 5 provides concluding remarks and some recommendations.

2.   Features and Summary of Data

To begin with, it would be in order to describe the data that have been used in this analysis. In particular, the SAE analysis is based on the AIDIS 2012-13 data for rural areas of the State of Karnataka in India and the Population Census of 2011. The sampling design used in the AIDIS 2012-13 data is stratified multi-stage random sampling with districts as strata, the census villages in the rural sector as first stage units and households as the ultimate stage units. For the state of Karnataka, there are a total of 2340 surveyed rural households (including both indebted and non-indebted) spread over 30 districts. The rural households are broadly classified into two types; namely; cultivator and non-cultivator households. As per the concepts and definitions of AIDIS, all rural households operating at least 0.002 hectare of land during the 365 days preceding the date of survey are treated as 'cultivator households'. On the other hand, all rural households operating no land or land less than 0.002 hectare are considered to be non-cultivator households. What follows, based on land holding size (LHS), we denote three categories of households: (i) LHS-A: All households (ii) LHS-C: Cultivator-households with LHS greater than 0.002 ha, and (iii) LHS-NC: Non cultivator-households with LHS less or equal to 0.002 ha. Here, the districts and district by household categories are small areas of interest. Table 1 presents the distribution of district-wise sample sizes for three categories of households. Across all the districts (*i.e.* LHS-A), the sample size ranges between a minimum

of 55 households to a maximum of 112 with an average of 78 households. The sample sizes become too small if sub-grouped further by land holding size categories (i.e. district by cultivator and non-cultivator categories). That is, the sample size of rural cultivators (LHS-C) varies from a minimum of 23 to a maximum of 90 households across the 30 districts with an average of 49 households. And for non-cultivators (LHS-NC), the sample size varies from a minimum of 11 to a maximum of 51 households across the districts with an average of 29 households. Such small samples from the districts pose a challenge in deriving reliable direct estimates of indebtedness. Thus, SAE is an obvious choice to address this problem.

Table 1: Distribution of sample size by occupational categories across districts in rural Karnataka

District	All	Cultivator	Non-Cultivator	District	All	Cultivator	Non-Cultivator
Belgaum	112	67	45	Tumkur	112	90	22
Bagalkot	84	57	27	Kolar	56	45	11
Bijapur	112	85	27	Bangalore	56	23	33
Gulbarga	98	60	38	Bangalore Rural	56	34	22
Bidar	84	49	35	Mandya	112	85	27
Raichur	84	55	29	Hassan	84	63	21
Koppal	84	63	21	Dakshina Kannada	84	41	43
Gadag	56	31	25	Kodagu	56	35	21
Dharwad	56	28	28	Mysore	112	71	41
Uttara Kannada	56	32	24	Chamarajanagar	56	39	17
Haveri	84	52	32	Ramanagara	55	24	31
Bellary	112	72	40	Chikkaballapura	56	42	14
Chitradurga	84	33	51	Yadgir	56	44	12
Davanagere	84	58	26	Minimum	55	23	11
Shimoga	87	50	37	Maximum	112	90	51
Udupi	56	28	28	Average	78	49	29
Chikmagalur	56	27	29	Total	2340	1483	857

Two types of variables are utilized in SAE technique, the variable of interest and the auxiliary variable. As noticed in Section 1, the auxiliary (covariates) variables play an important role in SAE. The auxiliary variables for this analysis are available at district level from the Census 2011. The Population Census 2011 provides a number of covariates at district level that can be utilized for small area modeling. We therefore carried out a preliminary data analysis in order to define appropriate covariates for SAE modeling, using Principal Component Analysis (PCA) to derive composite scores for selected groups of variables. In particular, we carried out PCA separately on three groups of variables, all measured at district level and identified as P1, P2 and P3 below. The first group (P1) consisted of literacy rates by gender and proportions of worker population by gender. The first principal component (P11) for this group explained 61% of the variability, while adding the second principal component (P12) increased explained variability to 85%. The second group (P2) consisted of the proportions of main worker by gender, proportions of main cultivator by gender and proportions of main agricultural labourer by gender. The first principal component (P21) for this second group explained 48% of the variability in the P2 group, while adding the second component (P22) increased explained variability to 62%. Finally, the third group (P3) consisted of proportions of marginal cultivator by gender and proportions of marginal agriculture labourers by gender. The first principal component (P31) for this third group explained 37% of the variability in the P3 group, while adding the second component (P32) increased explained variability to 60%. Finally, three variables, P11, P21 and P31 that significantly explained the model with AIC value 51.59, are identified for the use in SAE analysis. In this paper, the *Y*-

variable of interest is the indebted households, i.e. whether a household is in debt or not. A household is defined to be indebted if it has outstanding loan (from respective source) as on 30.06.2012. The target is to estimate the proportion of indebted household (*i.e.* the incidence of indebtedness) at the district (LHS-A) and district by household category (LHS-C and LHS-NC) level. Incidence of indebtedness (IOI) is defined as number of households with any one loan (from respective source) divided by all households in that population segment.

3.   Methodological Framework

This Section describes the methodology used in the small area analysis considered in this paper. To begin with, we assume a finite population U of size N which is consisting of D non-overlapping and mutually exclusive small areas (or district in this paper). We assume that a sample s of size n is drawn from this population using a probability sampling method. Here, a subscript d has been used to denote quantities related to small area d. Let U_d and s_d be the population and sample of sizes N_d and n_d in area d, respectively such that $U = \bigcup_{d=1}^{D} U_d$, $N = \sum_{d=1}^{D} N_d$, $s = \bigcup_{d=1}^{D} s_d$ and $n = \sum_{d=1}^{D} n_d$. We use subscript s and r respectively to denote quantities related to sample and non-sample parts of the population. Let y_{di} denotes the value of the variable of interest for unit $i (i = 1,..., N_d)$ in area d. The variable of interest, with values y_{di}, is binary (*e.g.* $y_{di} = 1$ if i^{th} household is in debt and 0 otherwise) in area d, the aim is to estimate the small area population count, $y_d = \sum_{i \in U_d} y_{di}$, or equivalently the small area proportion, $P_d = N_d^{-1} y_d$, in area d. The standard direct survey estimator (hereafter denoted by DIR) for P_d is, $p_{dw} = \sum_{i \in s_d} \widetilde{w}_{di} y_{di}$ where $\widetilde{w}_{di} = \frac{w_{di}}{\sum_{i \in s_d} w_{di}}$ is the normalized survey weight with $\sum_{i \in s_d} \widetilde{w}_{di} = 1$ and w_{di} is the survey weight for unit i in area d. The estimated design-based variance of DIR is approximated by $v(p_{dw}) = \sum_{i \in s_d} \widetilde{w}_{di} (\widetilde{w}_{di} - 1)(y_{di} - p_{dw})^2$, with the simplifications $w_{di} = a_{di}^{-1}$, $a_{di,di} = a_{di}$ and $a_{di,dj} = a_{di} a_{dj}, i \neq j$, where a_{di} is the first order inclusion probability of unit i in area d and $a_{di,dj}$ is the second order inclusion probability of units i and j in area d. Under simple random sampling (SRS), $w_{di} = N_d n_d^{-1}$ and DIR is then $p_d = n_d^{-1} y_{sd}$, with estimated variance $v(p_d) \approx n_d^{-1} p_d (1 - p_d)$, where $y_{sd} = \sum_{i \in s_d} y_{di}$ denotes the sample count in area d. Similarly, $y_{rd} = \sum_{i \in s_r} y_{di}$ denotes the non-sample count in area d. If the sampling design is informative, this SRS-based version of DIR may be biased. Furthermore, DIR is based on area-specific sample data and can therefore be very imprecise when the area specific sample size is small or may even be impossible to compute if this sample size is zero. However, model-based SAE procedures that 'borrow strength' via a common statistical model for all the small areas can be used to address this problem. If we ignore the sampling design, the sample count y_{sd} in area (*i.e.* district) d can be assumed to follow a Binomial distribution with parameters n_d and π_d, *i.e.* $y_{sd} = Bin(n_d, \pi_d)$, where π_d is the probability of occurrence of an event for a population

unit in area d or the probability of prevalence in area d. Similarly, for the non-sample count, $y_{rd} \sim Bin(N_d - n_d, \pi_d)$. Further, y_{sd} and y_{rd} are assumed to be independent binomial variables with π_d being a common success probability.

Let $\mathbf{x}_d$ be the k-vector of covariates for area d from available data sources. Following Chandra *et al.* (2011) the model linking the probability π_d with the covariates $\mathbf{x}_d$ is the logistic linear mixed model of the form

$$logit(\pi_d) = \ln\left\{\pi_d(1-\pi_d)^{-1}\right\} = \eta_d = \mathbf{x}_d^T\boldsymbol{\beta} + u_d, \tag{1}$$

with $\pi_d = \exp(\mathbf{x}_d^T\boldsymbol{\beta} + u_d)\left\{1 + \exp(\mathbf{x}_d^T\boldsymbol{\beta} + u_d)\right\}^{-1}$. Here $\boldsymbol{\beta}$ is the k-vector of regression coefficients, often known as fixed effect parameters, and u_d is the area-specific random effect that captures the area dissimilarities. We assume that u_d's are independently and normally distributed with mean zero and variance σ_u^2. Here, we observe that model (1) relates the area level proportions (direct estimates) from the survey data to the area level covariates. The Fay and Herriot (FH) method for SAE is based on area level linear mixed model and their approach is applicable to a continuous variable. Model (1), a special case of a generalized linear mixed model (GLMM) with logit link function, is suitable for modelling discrete data, particularly the binary variables. (Chandra, 2013; Chandra *et al.*, 2017). Under model (1), an empirical predictor (EP) of the population count y_d in area d is

$$\hat{y}_d^{EP} = y_{sd} + \hat{y}_{rd} = y_{sd} + (N_d - n_d)\left[\exp(\mathbf{x}_d^T\hat{\boldsymbol{\beta}} + \hat{u}_d)\left(1 + \exp(\mathbf{x}_d^T\hat{\boldsymbol{\beta}} + \hat{u}_d)\right)^{-1}\right]. \tag{2}$$

An estimate of the corresponding proportion in area d is obtained as $\hat{p}_d^{EP} = N_d^{-1}\hat{y}_d^{EP}$. It is obvious that in order to compute the small area estimates by equation (2), we require estimates of the unknown parameters $\boldsymbol{\beta}$ and $\mathbf{u} = (u_1, ..., u_D)^T$. We can observe that the parameters $\boldsymbol{\beta}$ and σ_u^2 are the same for every area; *i.e.*, they can be estimated using the data from all small areas. We use an iterative procedure that combines the Penalized Quasi-Likelihood (PQL) estimation of $\boldsymbol{\beta}$ and $\mathbf{u}$ with REML estimation of σ_u^2 to estimate unknown parameters (Chandra *et al.*, 2011).

The mean squared error (MSE) estimates are computed to assess the reliability of estimates and also to construct the confidence interval (CI). The MSE estimate of (2) is:

$$mse(\hat{p}_d^{EP}) = M_1(\hat{\sigma}_u^2) + M_2(\hat{\sigma}_u^2) + 2M_3(\hat{\sigma}_u^2). \tag{3}$$

Following Chandra *et al.* (2011) we define few notations to express different components of (3). We denote by $\hat{\mathbf{V}}_s = diag\left\{n_d\hat{p}_d^{EP}(1-\hat{p}_d^{EP})\right\}$ and $\hat{\mathbf{V}}_r = diag\left\{(N_d - n_d)\hat{p}_d^{EP}(1-\hat{p}_d^{EP})\right\}$ the diagonal matrices defined by the corresponding variances of the sample and non-sample parts, respectively. We then define $\mathbf{A} = \left\{diag(N_d^{-1})\right\}\hat{\mathbf{V}}_r$, $\mathbf{B} = \left\{diag(N_d^{-1})\right\}\hat{\mathbf{V}}_{rd}\mathbf{X} - \mathbf{A}\hat{\mathbf{T}}\hat{\mathbf{V}}_s\mathbf{X}$ and

$\hat{\mathbf{T}} = \left(\hat{\sigma}_u^2 \mathbf{I}_D + \hat{\mathbf{V}}_s \right)^{-1}$, where $\mathbf{X} = (\mathbf{x}_1^T, ..., \mathbf{x}_D^T)^T$ is a $D \times k$ matrix, and $\mathbf{I}_D$ is an identity matrix of order D. We further write $\hat{\mathbf{T}}_{11} = \left\{ \mathbf{X}^T \hat{\mathbf{V}}_s \mathbf{X} - \mathbf{X}^T \hat{\mathbf{V}}_s \hat{\mathbf{T}} \hat{\mathbf{V}}_s \mathbf{X} \right\}^{-1}$ and $\hat{\mathbf{T}}_{22} = \hat{\mathbf{T}} + \hat{\mathbf{T}} \hat{\mathbf{V}}_s \mathbf{X} \hat{\mathbf{T}}_{11} \mathbf{X}^T \hat{\mathbf{V}}_s^T \hat{\mathbf{T}}$. Under model (1), the components of MSE estimate are: $M_1(\hat{\sigma}_u^2) = \mathbf{A} \hat{\mathbf{T}} \mathbf{A}^T$, $M_2(\hat{\sigma}_u^2) = \mathbf{B} \hat{\mathbf{T}}_{11} \mathbf{B}^T$ and $M_3(\hat{\sigma}_u^2) = trace \left(\hat{\nabla}_i \hat{\mathbf{\Sigma}} \hat{\nabla}_j' v(\hat{\sigma}_u^2) \right)$ with $\hat{\mathbf{\Sigma}} = \hat{\mathbf{V}}_{sd} + \hat{\phi} \mathbf{I}_D \hat{\mathbf{V}}_{sd} \hat{\mathbf{V}}_{sd}^T$. Let us write $\Delta = \mathbf{A} \hat{\mathbf{T}}$ and $\hat{\nabla}_i = \partial(\Delta_i)/\partial \phi \big|_{\phi = \hat{\phi}} = \partial(A_i \hat{\mathbf{T}})/\partial \sigma_u^2 \big|_{\sigma_u^2 = \hat{\sigma}_u^2}$, where A_i is the ith row of the matrix A. Here $v(\hat{\sigma}_u^2)$ is the asymptotic covariance matrix of the estimate of variance component $\hat{\sigma}_u^2$, which can be evaluated as the inverse of the appropriate Fisher information matrix for $\hat{\sigma}_u^2$. This term also depends upon whether we use ML or REML estimate of $\hat{\sigma}_u^2$. We use REML estimates for $\hat{\sigma}_u^2$ and where $v(\hat{\sigma}_u^2) = 2 \left((\hat{\sigma}_u^2)^{-2} (D - 2t_1) + (\hat{\sigma}_u^2)^{-4} t_{11} \right)^{-1}$ with $t_1 = (\hat{\sigma}_u^2)^{-1} trace(\hat{\mathbf{T}}_{22})$ and $t_{11} = trace(\hat{\mathbf{T}}_{22} \hat{\mathbf{T}}_{22})$.

4.   Model Settings and Estimators

The semi-parametric or the non-parametric covariance model considered for the study is of the form

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \phi(\mathbf{U}) + \boldsymbol{\varepsilon} \tag{4}$$

where, $\mathbf{Y}$ is the observation vector, $\mathbf{m} = \mathbf{X}\boldsymbol{\beta} + \phi(\mathbf{U})$, is the regression function, $\mathbf{X}$ is the design matrix, $\boldsymbol{\beta}$ is the vector of treatment effect, $\phi(\mathbf{U})$ is the non-parametric function representing the relationship between $\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}$ and the covariate $\mathbf{U}$ which is assumed to be a smooth function and $\boldsymbol{\varepsilon}$ is the error term assumed to be *iid* with mean vector $\mathbf{0}$ and covariance matrix $\sigma^2 \mathbf{I}$. Back-fitting algorithm (Buja *et al.*, 1989) is used to estimate the treatment vector and covariate effect in the regression model and estimates are given by

$$\hat{\boldsymbol{\beta}} = [\mathbf{X}^T(\mathbf{I} - \mathbf{S})\mathbf{X}]^{-1}\mathbf{X}^T(\mathbf{I} - \mathbf{S})\mathbf{Y}, \quad \hat{\boldsymbol{\phi}} = \mathbf{S}(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \quad \text{and} \quad \hat{\mathbf{m}} = \mathbf{X}\hat{\boldsymbol{\beta}} + \hat{\boldsymbol{\phi}}$$

where, $\mathbf{S}$ is the smoothing matrix derived using local linear regression (Ruppert and Wand, 1994). Let $\mathbf{S}_i$ be the ith row of the smoother matrix, then

$$\mathbf{S} = [\mathbf{S}_1 \, ... \, \mathbf{S}_n]^T$$
$$\mathbf{S}_i^T = \mathbf{e}_1^T \left(\mathbf{Z}_{u_i}^T \mathbf{W}_{u_i} \mathbf{Z}_{u_i} \right)^{-1} \mathbf{Z}_{u_i}^T \mathbf{W}_{u_i}$$

where,

$$\mathbf{Z}_{u_i} = \begin{bmatrix} 1 & (u_1 - u_i) \\ \vdots & \vdots \\ 1 & (u_n - u_i) \end{bmatrix}, \quad \mathbf{e}_1^T = [1 \ 0 \ 0]$$

and $\mathbf{W}_{u_i} = diag \left\{ K \left(\frac{u_1 - u_i}{h} \right), ..., K \left(\frac{u_n - u_i}{h} \right) \right\}$ for some kernel functions K and bandwidth h. The properties of the estimates are provided by Jose and Ismail (2001) and Rupert and Wand (1994). Cross-validation (leave-one-out) technique is generally used to estimate the optimum bandwidth h. The cross-validation score is given by

$$CV(h) = \frac{1}{n}\sum_{i=1}^{n}\left[y_i - \hat{m}_{(-i)h}\right]^2$$

where, y_i, $i = 1,\ldots,n$ are the observations and $\hat{m}_{(-i)h}$ is the leave-one-out estimate (estimated value of m_i without using the ith observation) with h as bandwidth. The optimum bandwidth is the value of h which minimizes the cross-validation score $CV(h)$. The estimate, $\hat{\boldsymbol{\beta}}$ is asymptotically unbiased and its asymptotic variance is $\sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$ which is same as the fully parametric model (Opsomer and Ruppert, 1999). Cleveland and Devlin (1988) and Hastie and Tibshirani (1990) discussed the estimation of error variance in linear regression smoothers. An approximate estimate of the error variance is given by

$$\hat{\sigma}^2 = \frac{1}{[n - p - 2trace(\mathbf{S}) + trace(\mathbf{S}^T\mathbf{S})]}\left[\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\phi}}\right]^T\left[\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\phi}}\right]$$

The variance of $\hat{\boldsymbol{\beta}}$ is estimated by

$$\hat{V}\left(\hat{\boldsymbol{\beta}}\right) = diag(\mathbf{P}\mathbf{P}^T)\hat{\sigma}^2$$

where, $\mathbf{P} = (\mathbf{X}^T(\mathbf{I}\text{-}\mathbf{S})\,\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{I}\text{-}\mathbf{S})$. The significance of the covariate effect $\boldsymbol{\phi}$ can be tested using the lack of fit statistic or by comparing the mean residual sum of squares (Hart, 1997; Jose, *et al.*, 2009). Under the null hypothesis that the covariate effect $\phi(\mathbf{U}) = \mathbf{0}$, the mean residual sum of squares obtained by fitting the model (1) is given by

$$\hat{\sigma}_0^2 = \mathbf{Y}^T[\mathbf{I} - \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}]^T[\mathbf{I} - \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}]\mathbf{Y}/(n - p - 1)$$

The lack of fit statistic is given by

$$R = \frac{\hat{\sigma}_0^2}{\hat{\sigma}^2}$$

The statistic R asymptotically follows an F distribution with $(n-p-1)$, $[n-p-2trace(\mathbf{S})+ trace(\mathbf{S}^T\mathbf{S})]$ degrees of freedom and it can be used for testing the significance of the covariate effect.

5. Analysis of Data in the Presence of Outliers

The regression estimate and the cross-validation technique can behave very badly in the presence of outliers in the data or when the errors are heavy-tailed (Leung, D., 2005). One remedy is to remove the influential observations from the data. Another approach is to use robust smoother, which is not as vulnerable as the usual smoothing technique. A robust M-type estimate $\hat{m}$ of the regression function can be obtained by minimizing the objective function

$$\sum_{i=1}^{n}\rho\left[\frac{y_i - \hat{m}_i}{s}\right] \tag{5}$$

where, $\rho(.)$ is an even function with bounded first derivative $\psi(.)$ and a unique minimum at zero. The derivative $\psi(x) = \dfrac{d\rho(x)}{dx}$ is called the influence function and $w(x) = \dfrac{\psi(x)}{x}$ is the corresponding weight function. Several M-type estimators have been discussed in literature using different types of influence functions (Huber, 1981; Rey, 1983; Hampel *et al.*, 1986; Tukey, 1977). Tuckey's bi-weight robust function is very popular and it is considered in this paper. The ρ, ψ and w functions corresponding to the Tuckey's robust estimator is given by

$$\rho(x) \quad = \begin{cases} \frac{c^2}{6}\left[1 - \left(1 - \left(\frac{x}{c}\right)^2\right)\right]^3 & |x| \le c \\ \frac{c^2}{6} & |x| > c \end{cases}$$

$$\psi(x) = \begin{cases} x\left[\left(1 - \left(\frac{x}{c}\right)^2\right)\right]^2 & |x| \le c \\ 0 & |x| > c \end{cases}$$

$$w(x) = \begin{cases} \left[\left(1 - \left(\frac{x}{c}\right)^2\right)\right]^2 & |x| \le c \\ 0 & |x| > c \end{cases}$$

The turning constant c is picked to give reasonably high efficiency. When the errors are normal and x is the standardized residual, then $c = 4.685$ produce 95% efficiency.
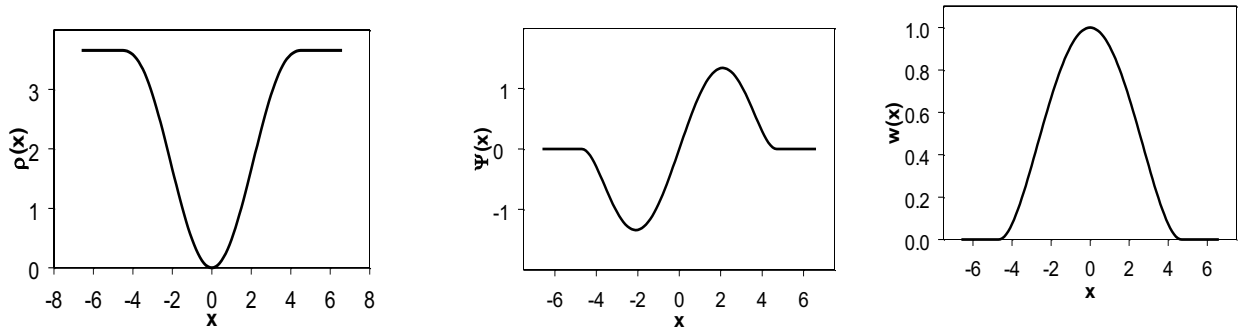

Figure 1: ρ, ψ and w functions of Tuckey's bi-weight robust estimate

Iterated reweighted least squares technique is used to solve the minimization problem in eq. (2) to obtain the robust estimate of the regression function. The estimate of the regression function in the kth iteration is given by

$$\widehat{\mathbf{m}}_{(k)} = \mathbf{X}\widehat{\boldsymbol{\beta}}_{(k)} + \widehat{\boldsymbol{\phi}}_{(k)}$$

$$\widehat{\boldsymbol{\beta}}_{(k)} = \left[\mathbf{X}^T(\mathbf{I} - \mathbf{S}_{(k)})\mathbf{X}\right]^{-1}\mathbf{X}^T(\mathbf{I} - \mathbf{S}_{(k)})\mathbf{Y}$$

$$\widehat{\boldsymbol{\phi}}_{(\mathbf{k})} = \mathbf{S}_{(k)}\left(\mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_{(k)}\right)$$

where, $\mathbf{S}_{(k)}$ is the smoothing matrix in the kth iteration derived using robust local linear regression. Let $\mathbf{S}_{i(k)}$ be the ith row of the smoothing matrix in the kth iteration, then

$$\mathbf{S}_{(k)} = \left[\mathbf{S}_{1(k)} \cdots \mathbf{S}_{n(k)}\right]^T$$

$$\mathbf{S}_{i(k)}^T = \boldsymbol{e}_1^T\left(\mathbf{Z}_{u_i}^T\mathbf{W}_{u_i(k)}^*\mathbf{Z}_{u_i}\right)^{-1}\mathbf{Z}_{u_i}^T\mathbf{W}_{u_i(k)}^*$$

$$\mathbf{W}^*_{u_i(k)} = diag\{w^*_i(r_{1(k-1)}), \dots, w^*_i(r_{n(k-1)})\}$$

$$w^*_i(r_{j(k-1)}) = \frac{K\left(\frac{u_i - u_j}{h}\right) w(r_{j(k-1)})}{\sum_{l=1}^n K\left(\frac{u_i - u_l}{h}\right) w(r_{l(k-1)})} , \qquad j = 1, \dots, n$$

where $w(r_{j(k-1)})$ is the value of the robustness weight function corresponding to y_j in the kth iteration and $r_{(k-1)j} = \frac{[y_j - \hat{m}_{j(k-1)}]}{s_{(k-1)}}$ is the standardized residual of the jth datum in the $(k-1)^{th}$ iteration with $\hat{m}_{j(k-1)}$ as the estimated value and $r_{(0)i} = 0$ for $i = 1, \dots, n$. The Median of Absolute Deviation from median (*MAD*) is used for computing a robust estimate for the scale factor s and

$$s_{(k-1)} = \frac{median_i \left| e_{(k-1)i} - median_j(e_{(k-1)j}) \right|}{0.6745}$$

where $e_{(k-1)i} = y_i - \hat{m}_{i(k-1)}$

The estimate of the regression function in the kth iteration is written as

$$\hat{\mathbf{m}}_{(k)} = \mathbf{X}\hat{\boldsymbol{\beta}}_{(k)} + \mathbf{S}_{(k)}(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{(k)})$$

Iteration is continued till there is no significant improvement in the estimated values and the final estimate of the regression function is written as

$$\hat{\mathbf{m}}^* = \mathbf{X}\hat{\boldsymbol{\beta}}^* + \mathbf{S}^*(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}^*)$$
$$\hat{\boldsymbol{\beta}}^* = [\mathbf{X}^T(\mathbf{I} - \mathbf{S}^*)\mathbf{X}]^{-1}\mathbf{X}^T(\mathbf{I} - \mathbf{S}^*)\mathbf{Y}$$
$$V(\hat{\boldsymbol{\beta}}^*) = diag(\mathbf{P}^*\mathbf{P}^{*T})\hat{\sigma}^{*2}$$

where $\mathbf{S}^*$ is the smoothing matrix of the final iteration, $\hat{\mathbf{m}}^*$, $\hat{\boldsymbol{\beta}}^*$ and $\hat{\sigma}^*$ are the final estimates of the regression function, treatment vector and scale factor respectively and

$$\mathbf{P}^* = (\mathbf{X}^T(\mathbf{I}-\mathbf{S}^*)\,\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{I}-\mathbf{S}^*)$$

Optimum bandwidth: Let $w^{\#}_i$ be the final robustness weight assigned to y_i and $\hat{m}^{\#}_{i(h)}$ be the estimated value of m_i with band width h. The Mean Squared Error (*MSE*) of the estimated value corresponding to the bandwidth h is given by

$$MSE(h) = \frac{1}{n}\sum_{i=1}^n (y_i - \hat{m}^{\#}_{i(h)})^2$$

The cross-validation score *CV* (h) does not work well for the robust smoothers because the *CV* function itself is strongly influenced by the outliers (Wang and Scott, 1994). The cross-validation score is the sum of squares of the prediction errors of the smoother at each of the design points. When there are outliers, the prediction errors corresponding to the outliers will be uncharacteristically extreme and these extreme prediction errors will inflate the *CV*(h).

Therefore, similar to robust smoothing technique, the influence of extreme prediction errors should be minimized. A robust cross validation score $RCV(h)$ is defined as

$$RCV(h) = \frac{\sum_{i=1}^{n} w_i^{\#} \left(y_i - \widehat{m}_{(-i)(h)}^{\#} \right)^2}{\sum_{i=1}^{n} w_i^{\#}}$$

where, $w_i^{\#}$ is the final robustness weight defined earlier, $\widehat{m}_{(-i)(h)}^{\#}$ is the robust estimate of y_i with h as bandwidth and without using the ith observation y_i. The value of h which minimizes the robust cross validation score $RCV(h)$ will be the optimum bandwidth. In the computation of $RCV(h)$, the effect of outliers is controlled by taking weighted sum of squares of the prediction errors of the smoother at each of the design points with the robustness weight $w_i^{\#}$.

6.   Simulation Study

A simulation study was conducted to evaluate the performance of the proposed method. The semi-parametric regression model considered for the simulation study is given by

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \phi(\mathbf{U}) + \boldsymbol{\varepsilon} \tag{6}$$

where $\mathbf{Y}$ is the $n \times 1$ observation vector, $\mathbf{m} = \mathbf{X}\boldsymbol{\beta} + \phi(\mathbf{U})$, is the regression function, $\mathbf{X}$ is the $n \times k$ design matrix, $\boldsymbol{\beta}$ is the $k \times 1$ treatment effect vector which is taken as $\boldsymbol{\beta}^T = [-2\ -2\ 0\ 4]$, $\phi(u) = 1 + 2sin(\pi u)$ and the random error vector $\boldsymbol{\varepsilon}$ follows $N(\mathbf{0}, \sigma^2 \mathbf{I})$ and $u \in [0,1]$. Based on the above, 100 sets of data are simulated for different values of n (100, 200, 400) and σ (1.0, 2.0) with 0%, 4% and 8% outliers. To generate data with specific percentage of outliers, the required number of random numbers between 0 to n are generated and the value of the regression function m corresponding to the data points are replaced with $m+6\sigma$. The Epanechnikov kernel function $K(u) = 0.75(1-u^2)$ is employed in the study. The treatment effect vector $\boldsymbol{\beta}^T = [\beta_1\ \beta_2\ \beta_3\ \beta_4]$, the nonparametric functi

on ϕ and the error variance σ^2 are estimated using the method given in Section 2. Tuckey's bi-weight function with the turning point $c=4.685$ is used as the robustness function. The Average Mean Squared Errors ($AMSE$) of the estimated values of σ, $\boldsymbol{\beta}$, ϕ and $\mathbf{m}$ with the true values of 100 sets of simulated data for different values of n (100, 200, 400) and σ (1.0, 2.0) are given in Table A.2. The $AMSE$ of the estimated parameters are calculated as follows:

$$AMSE \text{ of } \widehat{\sigma} = \frac{1}{100} \sum_{i=1}^{100} \left(\sigma - \widehat{\sigma}_{(i)} \right)^2,$$

$$AMSE \text{ of } \widehat{\boldsymbol{\beta}} = \sum_{j=1}^{4} \frac{1}{100} \sum_{i=1}^{100} \left(\beta_j - \widehat{\beta}_{j(i)} \right)^2$$

$$AMSE \text{ of } \widehat{\boldsymbol{\phi}} = \frac{1}{100} \sum_{i=1}^{100} \frac{1}{n} \sum_{j=1}^{n} \left[\phi(u_j) - \widehat{\phi}_{(i)}(u_j) \right]^2,$$

$$AMSE \text{ of } \widehat{\mathbf{m}} = \frac{1}{100} \sum_{i=1}^{100} \frac{1}{n} \sum_{j=1}^{n} \left[m - \widehat{m}_{(i)}(u_j) \right]^2$$

where, $\widehat{\sigma}_{(i)}$, $\widehat{\beta}_{j(i)}$, $\widehat{\phi}_{(i)}$ and $\widehat{m}_{(i)}$ are the estimated values of σ, β_j, ϕ and the regression function m corresponding to the ith simulated data set. The bias of the point estimates of $\widehat{\sigma}, \widehat{\beta}_j, j = 1,\ldots,4$ are calculated as follows

$$\text{Bias of } \hat{\sigma} = \frac{1}{100} \sum_{i=1}^{100} \left(\sigma - \hat{\sigma}_{(i)} \right)$$

$$\text{Bias of } \hat{\beta}_j = \frac{1}{100} \sum_{i=1}^{100} \left(\beta_j - \hat{\beta}_{j(i)} \right), j=1,\dots,4$$

The *AMSE* of the estimates are converging to zero as *n* increases or in other words, the estimated values are converging to the true values as *n* increases. Note that the bias of the point estimates $\hat{\sigma}, \hat{\beta}_j$, *j* = 1,…,4 are also negligible as *n* increases (Table A.2). This indicates the consistency of the estimates. The *MSE* varies with change in the choice of bandwidths. The optimum bandwidth (bandwidth corresponds to the minimum *MSE*) depends on the curvature of the function. The optimum bandwidth for estimating the parameters of the model was obtained based on the robust cross validation technique given in Section 2.

The comparison of Average Mean Squared Errors (*AMSE*) of the estimated values of σ, β, ϕ and **m** with the true values of 100 sets of simulated data for different values of *n* (100, 200, 400) and σ (1.0, 2.0) showed that in the presence of outliers (4% and 8%) the robust method performs much better than the non-robust method. The value of *AMSE* decreases as *n* increases or in other words the estimates converges to the true value.

Acknowledgements

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Appendix A

Table A.1: Optimum bandwidth ad *AMSE* of the estimates in the simulation study

σ	Outliers (%)	n	h	$AMSE(\widehat{\beta})$		$AMSE(\widehat{\phi})$		$AMSE(\widehat{m})$		$AMSE(\hat{\sigma})$	
				SP	Robust SP	SP	Robust SP	SP	Robust SP	SP	Robust SP
1	0	10	0.3	0.148	0.1471	0.079	0.0541	0.073	0.0664	0.006	0.0182
		20	0.2	0.072	0.0740	0.030	0.0256	0.039	0.0389	0.003	0.0078
		40	0.1	0.031	0.0341	0.016	0.0148	0.021	0.0218	0.001	0.0033
	4	10	0.3	0.371	0.1741	0.094	0.0608	0.183	0.0810	0.319	0.0143
		20	0.2	0.165	0.0849	0.052	0.0308	0.104	0.0408	0.308	0.0080
		40	0.1	0.077	0.0384	0.045	0.0162	0.094	0.0241	0.294	0.0038
	8	10	0.2	0.513	0.1793	0.244	0.0594	0.401	0.0846	0.882	0.0180
		20	0.2	0.228	0.0985	0.170	0.0285	0.272	0.0439	0.851	0.0133
		40	0.2	0.125	0.0548	0.144	0.0179	0.222	0.0231	0.833	0.0121
2	0	10	0.3	0.539	0.5672	0.191	0.1591	0.263	0.2588	0.018	0.0644
		20	0.3	0.300	0.3142	0.114	0.0887	0.145	0.1452	0.010	0.0415
		40	0.2	0.146	0.1530	0.054	0.0401	0.068	0.0674	0.004	0.0125
	4	10	0.3	1.469	0.6348	0.374	0.1797	0.742	0.2981	1.280	0.0432
		20	0.3	0.567	0.2865	0.213	0.0931	0.395	0.1386	1.229	0.0281
		40	0.2	0.323	0.1418	0.245	0.0509	0.357	0.0810	1.191	0.0224
	8	10	0.3	1.769	0.6486	1.066	0.1936	1.606	0.3138	3.369	0.0716
		20	0.3	0.947	0.3266	0.691	0.0900	1.081	0.1394	3.364	0.0584
		40	0.2	0.433	0.1461	0.761	0.0442	0.979	0.0709	3.369	0.0576

SP: Semi- parametric

Table A.2: Bias of the robust point estimates in the simulation study

σ	Outliers (%)	n	h	Bias of				
				$\hat{\beta}_1$	$\hat{\beta}_2$	$\hat{\beta}_3$	$\hat{\beta}_4$	$\hat{\sigma}$
1	0	100	0.30	–0.0184	–0.0187	0.0201	0.0169	–0.0610

		200	0.20	−0.0182	−0.0157	0.0155	0.0185	−0.0282
		400	0.15	0.0026	−0.0053	0.0127	−0.0100	−0.0187
	4	100	0.30	−0.0232	0.0100	−0.0010	0.0143	0.0440
		200	0.25	−0.0161	0.0112	−0.0002	0.0051	0.0346
		400	0.15	0.0033	0.0019	−0.0004	−0.0048	0.0294
	8	100	0.30	−0.0002	0.0166	−0.0077	−0.0088	0.0851
		200	0.25	−0.0008	0.0093	−0.0084	0.0000	0.0789
		400	0.20	0.0010	0.0039	−0.0058	0.0010	0.0745
2	0	100	0.30	−0.0060	−0.0079	0.0055	0.0085	−0.1037
		200	0.25	−0.0090	0.0234	−0.0156	0.0013	−0.0586
		400	0.20	−0.0030	0.0040	−0.0060	0.0051	−0.0398
	4	100	0.30	0.0222	−0.0271	−0.0120	0.0168	−0.0558
		200	0.25	0.0131	−0.0135	−0.0110	0.0114	0.0490
		400	0.20	−0.0060	0.0184	−0.0088	−0.0037	0.0445
	8	100	0.30	−0.0132	0.0294	−0.0131	−0.0031	0.1248
		200	0.30	−0.0143	0.0292	−0.0061	−0.0089	0.1160
		400	0.25	−0.0117	0.0202	−0.0106	0.0020	0.1119

Table A.3: Estimated values with standard errors (weight of nuts) of the field data

Parameter	Linear		Semi-parametric		Robust Semi-	
	Estimate	SE	Estimate	SE	Estimate	SE
$\mu+\beta_1$	9.969	0.683	9.924	0.622	9.925	0.548
$\mu+\beta_2$	9.414	0.683	9.570	0.626	9.573	0.552
$\mu+\beta_3$	10.029	0.638	9.949	0.594	9.950	0.524
$\mu+\beta_4$	9.883	0.675	9.994	0.617	9.991	0.543
$\mu+\beta_5$	9.922	0.691	9.918	0.636	9.916	0.560
$\mu+\beta_6$	10.767	0.630	10.758	0.587	10.758	0.517
σ	4.317		4.312	-	3.803	-

μ: Overall mean

Table A.4: Estimated values with standard errors (number of nuts) of the field data

Parameter	Linear		Semi-parametric		Robust Semi-parametric	
	Estimate	SE	Estimate	SE	Estimate	SE
$\mu+\beta_1$	328.80	22.71	331.96	20.71	330.80	16.83
$\mu+\beta_2$	307.84	22. 70	308.87	20.70	308.85	16.83
$\mu+\beta_3$	331.13	21.12	334.87	19.62	336.45	15.95
$\mu+\beta_4$	332.86	22.40	336.57	20.45	337.32	16.63
$\mu+\beta_5$	324.32	22.91	315.21	21.27	313.69	17.29
$\mu+\beta_6$	370.57	20.87	374.34	19.35	374.71	15.72
σ	143.06		142.96		116.16	

μ: Overall mean

Appendix-B

Figure B.1: Estimated survival functions of fitted models—Chemotherapy group
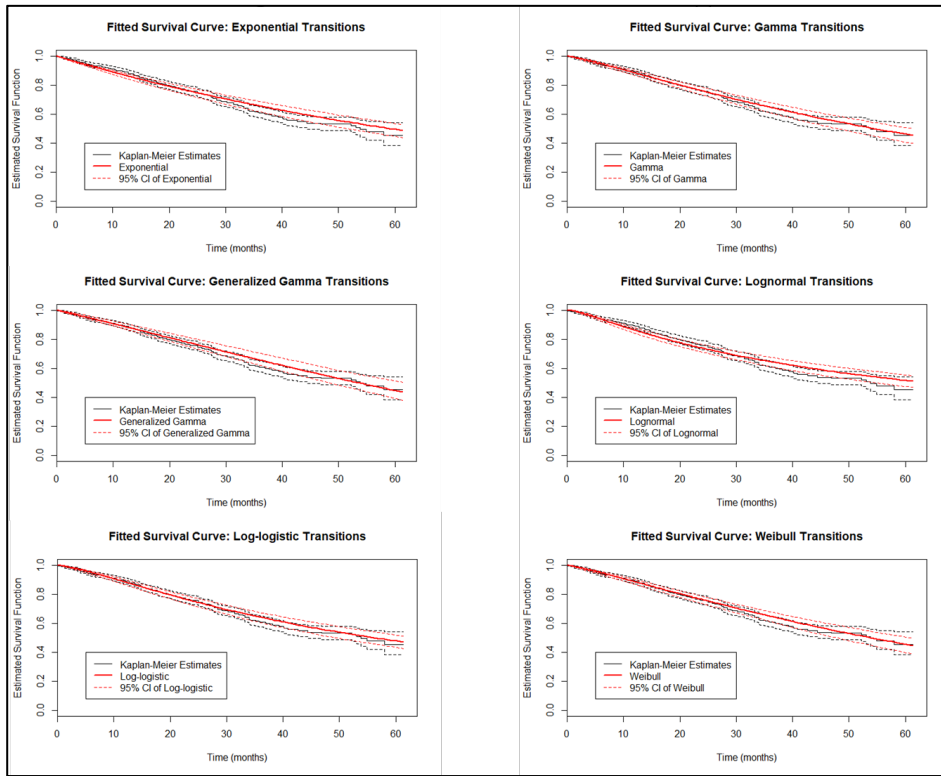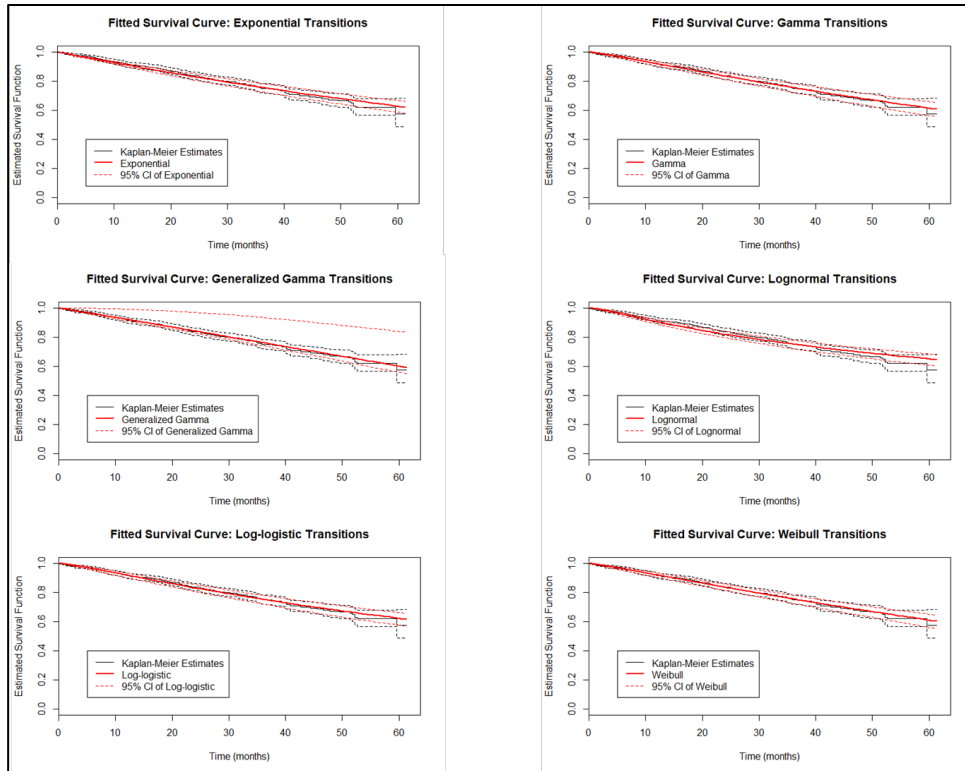

Figure B.2: Estimated survival functions of fitted models—Chemoimmunotherapy group

Appendix-C

Figure C.1: Transition probabilities plotted against time—Weibull semi-markov model
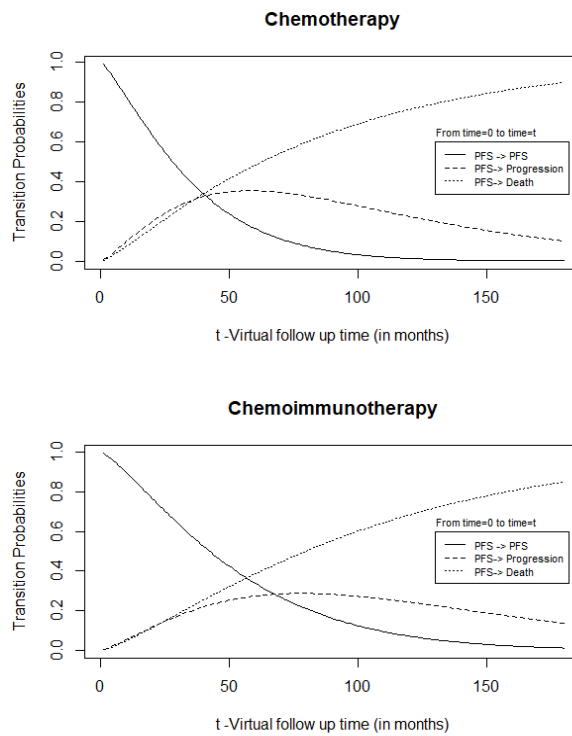

Figure C.2: Transition probabilities plotted against time—Multinomial-Dirichlet Bayesian model