

Robust model-based stratification sampling designs

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Abstract: We address the resistance, somewhat pervasive within the sampling community, to model-based methods. We do this by introducing notions of “approximate models” and then deriving sampling methods which are robust to model misspecification within neighbourhoods of the sampler’s approximate, working model. Specifically we study robust sampling designs for model-based stratification, when the assumed distribution $F_0(\cdot)$ of an auxiliary variable x , and the mean function and the variance function $g_0(\cdot)$ in the associated regression model, are only approximately specified. We adopt an approach of “minimax robustness,” to which end we introduce neighbourhoods of the “working” $F_0(\cdot)$, and working regression model, and maximize the prediction mean squared error (MSE) for the empirical best predictor, of a population total, over these neighbourhoods. Then we obtain robust sampling designs, which minimize an upper bound of the maximum MSE through a modified genetic algorithm with “artificial implantation.” The techniques are illustrated in a case study of Australian sugar farms, where the goal is the prediction of total crop size, stratified by farm size. *The Canadian Journal of Statistics* 43: 554–577; 2015 © 2015 Statistical Society of Canada

Résumé: Les auteurs tentent de diminuer la réticence généralisée de la communauté des méthodes d’enquête face aux méthodes d’échantillonnage basées sur un modèle en introduisant la notion de « modèle approximatif ». Ils en dérivent des méthodes d’échantillonnage robustes à la mauvaise spécification du modèle dans le voisinage d’un modèle approximatif mais fonctionnel de l’échantillonneur. Plus spécifiquement, les auteurs étudient les plans d’échantillonnage robustes pour la stratification basée sur un modèle lorsque la distribution $F_0(\cdot)$ d’une variable auxiliaire x et la fonction de variance $g_0(\cdot)$ du modèle de régression associé ne sont spécifiés qu’approximativement. Ils adoptent une approche de « robustesse minimax » pour laquelle ils définissent un voisinage « fonctionnel » de $F_0(\cdot)$ et un modèle de régression qui fonctionne, puis ils maximisent l’erreur quadratique moyenne de prévision (EQM) pour le meilleur prédicteur empirique du total de la population sur ces voisinages. Les auteurs obtiennent ainsi des plans d’échantillonnage robustes qui minimisent une borne supérieure de l’EQM grâce à un algorithme génétique modifié avec des « implantations artificielles ». Les auteurs illustrent leurs techniques par une étude de cas portant sur des fermes australiennes produisant du sucre et dont le but consiste à estimer la taille totale des récoltes à l’aide d’un échantillon stratifié selon la taille des fermes. *La revue canadienne de statistique* 43: 554–577; 2015 © 2015 Société statistique du Canada

1. INTRODUCTION

There is some, not inconsiderable, resistance within the sampling community to the use of model-based methods. A common reason for this is the reluctance of samplers to rely on methods whose

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efficacy declines sharply under model misspecification. In this article we aim to address this resistance as it affects model-based stratification methods; we do so by introducing model-robust methods whose performance is guaranteed not to drop below a bound determined by the level of uncertainty the sampler has in his or her working, approximate model. The methods are derived in the context of prediction of a population total, but can be extended to address other features of the target population.

Due to their non-homogeneity, populations such as those targeted in social or economic surveys are often divided into strata: distinct and non-overlapping subgroups. Generally desirable properties of strata are that they be large in size, differ considerably from one another, be internally homogeneous, and be such that the means of the target variable Y vary significantly across strata. In some cases, strata are “naturally defined”: for example, in household surveys strata may be states or provinces, income groups, occupations, age groups, etc. In business surveys, strata may be industries. In other cases, there may be information on the population frame that allows us to stratify the population. Typically, this information consists of the known values of a q -dimensional auxiliary variable \mathbf{x} with population values $\mathbf{x}_1, \dots, \mathbf{x}_N$. From each of L strata a sample s_h , of pre-specified size $n_h \leq N_h$, N_h being the population size in the h^{th} stratum, is drawn independently. Here L, n_h, N_h ($h = 1, \dots, L$) are all fixed, as is $N = \sum_{h=1}^L N_h$. Then, the collection of these samples constitutes a stratified sample $s = \cup_{h=1}^L s_h$ with sample size $n = \sum_{h=1}^L n_h$. If a simple random sample selection scheme is used in each stratum, then the corresponding sample is called a *stratified random sample*.

As strata are made up of population elements that are homogeneous within the stratum and heterogeneous with respect to elements of other strata we may assume that in the h^{th} stratum:

$$E(y_i | i \in h) = \mu_h, \quad \text{VAR}(y_i | i \in h) = \sigma_h^2, \quad y_i, y_j \text{ independent (if } i \neq j).$$

Here $i \in h$ indicates that population unit i is in the h^{th} stratum. The sample mean of Y within each of the strata is an empirical best predictor of the corresponding stratum population mean; hence, the empirical best predictor T^{EB} of the overall population total $T = \sum_{i=1}^N Y_i$ is given by $T^{\text{EB}} = \sum_h N_h \bar{y}_{n_h}$. Here \bar{y}_{n_h} is the sample mean of Y in the h^{th} stratum. The prediction variance of T^{EB} is given by $\sum_h (N_h^2/n_h)(1 - n_h/N_h)\hat{\sigma}_{n_h}^2$ where $\hat{\sigma}_{n_h}^2 = \frac{1}{n_h} \sum_{i \in s_h} (y_i - \bar{y}_{n_h})^2$ is the unbiased estimator of the variance σ_h^2 of Y -values in the h^{th} stratum.

In the population that motivates this article, the auxiliary variable x is univariate (i.e., $q = 1$). The crucial question for stratification is the construction of the stratum boundaries b_1, b_2, \dots, b_{L-1} of the target variable Y based on the auxiliary variable x so that the mean square error of an estimator is minimized. Dalenius (1950) established equations based on a single continuous auxiliary variable x . The solution of the equations would be the optimum boundaries when the equations are solvable. The method of Dalenius (1950) can be thought to form L strata as follows: assuming that x is distributed as $F_0(\cdot)$, and choosing $L - 1$ points between 0 and 1:

$$0 = a_0 < a_1 < \dots < a_h < \dots < a_{L-1} < a_L = 1,$$

then

$$y_i \text{ lies in the } h^{\text{th}} \text{ strata provided } F_0(x_i) \in (a_{h-1}, a_h]. \quad (1)$$

Such points a_1, \dots, a_{L-1} will be chosen to minimize the prediction mean square error of an estimator for a population parameter, such as the population total T_y . As the equations derived by Dalenius are generally unsolvable, Dalenius & Hodges (1959) derived methods to find approximately optimum boundaries. See Horgan (2006) and references therein for more methods of constructing stratum boundaries, and Ghosh (1963) for optimum stratification with bivariate predictors. An obvious extension of (1) is to replace the intervals $(a_{h-1}, a_h]$ by suitable hypercubes $\{S_h\}$ partitioning $[0, 1]^q$, and to put y_i in stratum h if $F_0(\mathbf{x}_i) \in S_h$. In order to proceed more directly to our intended application we concentrate here on $q = 1$.

Another way to model heterogeneity in a population is to use separate versions of linear regression models linking the target variable Y and the auxiliary variable x in different strata. Suppose that the sampler assumes the validity of the following model:

$$Y_i = \alpha_h + \beta_h x_i + g_0^{1/2}(x_i) \varepsilon_i, \quad i \in h, \quad h = 1, \dots, L. \quad (2)$$

The stratification scheme for (2) uses F_0 . Here $g_0(x) > 0$, and $\varepsilon_1, \dots, \varepsilon_N$ are independent and identically distributed random variables with mean zero and variance σ^2 . Model (2) is more general than the model

$$E(y_i | i \in h) = \alpha_h + \beta_h x_i, \quad \text{VAR}(y_i | i \in h) = \sigma_h^2, \quad y_i, y_j \text{ independent (if } i \neq j)$$

studied in Chambers & Clark (2012, display 5.14). Special cases of model (2) have been studied by many researchers. Bethel (1989) studied some estimators in model-based stratification using a model similar to (2) with parameters independent of strata:

$$Y_i = \alpha + \beta x_i + g_0^{1/2}(x_i) \varepsilon_i, \quad i = 1, \dots, N. \quad (3)$$

Kott (1985) used the special case $g_0(x) \equiv 1$ of model (3). In Section 2 of this article we will allow for misspecifications in the mean structure in (2); these lead to different optimal choices of $\{x_1, \dots, x_n\}$.

Assume that the method of sampling is non-informative. Then the regression model in the population also applies in the sample s with sample size n . Assume also that there is a complete response, so that once the sample has been selected and the in-sample units observed, the values of Y_i , $i \in s$ are known. Then we can use the values of Y_i , $i \in s$ and x_1, \dots, x_N to estimate or predict the finite population total $T = \sum_{i=1}^N Y_i$. The *design problem* is to specify a rule using x_1, \dots, x_N to select a sample s so that the estimator/predictor \hat{T} is optimal in that it minimizes a loss function such as the mean squared error (MSE) $E(T - \hat{T})^2$.

In the first method of modelling heterogeneity, the distribution function (d.f.) $F_0(\cdot)$ will typically only approximate reality. When the auxiliary variables are themselves subject to error (such as imperfect measurement), the problems of non-response adjustment were addressed by West & Little (2013). In such cases, the sampler might adopt the empirical distribution of the sampled auxiliary variables (for instance) as a “working distribution” $F_0(\cdot)$. However he or she should still entertain the possibility that more precise measurements might yield a d.f. F , more appropriate for purposes of stratification, which is unequal to, but in a neighbourhood of, the working distribution $F_0(\cdot)$. In the second method of modelling heterogeneity, the assumed mean function $\alpha_h + \beta_h x_i$ and variance function $g_0(\cdot)$ may be misspecified. We shall refer to them together as a working regression model and individually as a working mean function and a working variance function. We then construct robust sampling designs which give good results both at and “near” this working distribution and this working regression model.

The philosophy behind model robustness is that the experimenter/sampler will use his or her preferred methods and models, while seeking protection against increased loss if his or her choices turn out to be incorrect. Thus, the sampler fits his or her assumed mean and variance functions, and the stratum boundaries are determined by his or her choice F_0 . The effect of F is to determine the overall sample which is stratified prior to carrying out the analysis. These steps cannot be carried out in isolation from each other, hence our procedures are iterative.

Welsh & Wiens (2013) developed robust, model-based designs for a general class of models which includes the ratio model as a special case. We here extend their work to the case of stratified sampling. General problems of robust (in some sense) extrapolation or prediction from linear models—of which model-based sampling design is an example—have been studied by Fang & Wiens (2000), who constructed designs to minimize the (maximized) mean square predicted error; see also Dette & Wong (1996) and Wiens & Xu (2008), who studied robustness properties

of optimal extrapolation designs. Some general remarks on model-based design strategies are given by Nedyalkova & Tillé (2008). A survey of robustness of design is in Wiens (2015).

In Section 2 of this article we define explicitly the neighbourhoods of the working distribution and working regression model. In Section 3 we calculate the MSE for the empirical best predictor under arbitrary distributions $F(\cdot)$, and arbitrary regression models. We then maximize this MSE over a neighbourhood of the working regression model. The resulting maximum is to be itself maximized over a neighbourhood of $F_0(\cdot)$. This turns out to be impractically difficult, and so we solve an approximating problem by first deriving an upper bound on the maximum over the regression model, and then maximizing this upper bound over a neighbourhood of $F_0(\cdot)$. In this way we obtain a final loss function to be minimized over the class of possible random samples within each stratum. This minimization is a complex numerical problem which we handle, in Section 4, via a genetic algorithm. We introduce a novel process of “artificial implantation” into this algorithm; this greatly accelerates its progress.

We go on to find optimal designs for the Sugar Farm population discussed by Chambers & Dunstan (1986). We find that the robust designs give substantial protection against model misspecifications of the type considered here, at a minimal cost in efficiency when the working model is in fact accurate—exactly what a robust procedure is intended to achieve.

Derivations of major mathematical results are in the Appendix. The MATLAB code for the computations of Section 4 is available from the authors.

2. NEIGHBOURHOOD STRUCTURES

Suppose that the population is divided into L strata by applying (1). Denote by $\mathbf{Id}_h = (Id_{h1}, \dots, Id_{hN})'$ the indicator vector of the h^{th} stratum: $Id_{hi} = 1$ when $i \in h$ and $= 0$ otherwise. Define $\mathbf{x}_N = (x_1, \dots, x_N)'$ and $\mathbf{Z}_N = (\mathbf{Id}_1, \mathbf{Id}_1 * \mathbf{x}_N, \dots, \mathbf{Id}_L, \mathbf{Id}_L * \mathbf{x}_N) : N \times 2L$, where $*$ denotes the pointwise product of two vectors, and the parameters in the working regression model (2) are grouped as $\boldsymbol{\theta} = (\alpha_1, \beta_1, \dots, \alpha_L, \beta_L)^T$. Then we can rewrite (2) as

$$\mathbf{y}_N = \mathbf{Z}_N \boldsymbol{\theta} + \mathbf{G}_{0,N}^{1/2} \boldsymbol{\varepsilon}_N, \quad (4)$$

with $\mathbf{y}_N = (y_1, \dots, y_N)'$, $\boldsymbol{\varepsilon}_N = (\varepsilon_1, \dots, \varepsilon_N)'$, and $\mathbf{G}_{0,N} = \text{diag}\{g_0(x_1), \dots, g_0(x_N)\}$.

Suppose that, instead of the working regression model (4), the true regression model is now

$$\mathbf{y}_N = \mathbf{Z}_N \boldsymbol{\theta} + \boldsymbol{\psi}_N + \mathbf{G}_N^{1/2} \boldsymbol{\varepsilon}_N, \quad (5)$$

where $\boldsymbol{\psi}_N = (\psi(x_1), \dots, \psi(x_N))'$ represents a departure from the linear mean function and $\mathbf{G}_N = \text{diag}\{g(x_1), \dots, g(x_N)\}$, where $g(\cdot)$ is the appropriate variance function. The “true” parameter is defined by $\boldsymbol{\theta} = \arg \min_{\boldsymbol{\theta}} (E[\mathbf{y}_N] - \mathbf{Z}_N \boldsymbol{\theta})^2$, and then $\boldsymbol{\psi}_N =: E[\mathbf{y}_N] - \mathbf{Z}_N \boldsymbol{\theta}$ satisfies the orthogonality requirement $\mathbf{Z}_N' \boldsymbol{\psi}_N = \mathbf{0}$. We consider all $\boldsymbol{\psi}_N$ in the set

$$\Psi = \{\boldsymbol{\psi}_N : \mathbf{Z}_N' \boldsymbol{\psi}_N = \mathbf{0}, \|\boldsymbol{\psi}_N\| \leq \tau\}$$

for $\tau > 0$. Here $\|\cdot\|$ is the Euclidean norm. Instead of the working variance function $g_0(\cdot)$, the appropriate variance function is $g(\cdot)$ which is positive and “close to” $g_0(\cdot)$, in that it belongs to the class

$$\mathcal{G} = \{g : \mathbb{R} \longrightarrow \mathbb{R}^+ : 0 < g(x)g_0^{-1}(x) \leq 1 + \tau_g^2\},$$

for a specified τ_g .

Suppose that the appropriate distribution of x is $F(\cdot)$, in a neighbourhood of the working distribution $F_0(\cdot)$. Then, $Id_{h,j}$ is Bernoulli distributed with parameter $p_{F,h} = P_F[(F_0^{-1}(a_{h-1}), F_0^{-1}(a_h))]$. With $\mathbf{p}_F := (p_{F,1}, \dots, p_{F,L})'$ we define the neighbourhood of $F_0(\cdot)$ to be

$$\mathcal{F} = \{\text{all distributions } F(\cdot) \text{ such that } \|\mathbf{p}_F - \mathbf{p}_{F_0}\| \leq \delta\},$$

for a specified $\delta > 0$. An equivalent definition, which we find somewhat more convenient, is obtained by defining $\mathbf{p}^0 = \mathbf{p}_{F_0}$,

$$\mathcal{P} = \{\mathbf{p} \mid \|\mathbf{p} - \mathbf{p}^0\| \leq \delta; \mathbf{p} \succsim \mathbf{0}, \mathbf{1}'_L \mathbf{p} = 1\}, \quad (6)$$

and then defining \mathcal{F} to consist of those distributions with $\mathbf{p}_F \in \mathcal{P}$. (We use $\mathbf{p} \succsim \mathbf{0}$ to denote elementwise non-negativity.)

Suppose that a stratified random sample $s = \cup_{h=1}^L s_h$, with sample size $n = \sum_{h=1}^L n_h$, is chosen. The empirical best predictor of the population total T is

$$\hat{T} = \sum_{i \in s} Y_i + \sum_{i \notin s} \hat{Y}_i,$$

where for $i \notin s$, \hat{Y}_i is an estimator of $E(Y_i | Y_j, j \in s, x_1, \dots, x_N)$. Under the working regression model (4) we can get $\hat{Y}_i, i \notin s$ as follows. Corresponding to the n in-sample units and the $N - n$ non-sample units, define \mathbf{Z}_n and \mathbf{Z}_{N-n} to be the $n \times 2L$ and $(N - n) \times 2L$ submatrices of \mathbf{Z}_N , and define $\mathbf{G}_{0,n}$ to be the $n \times n$ submatrix of \mathbf{G}_0 and \mathbf{G}_{N-n} to be the $(N - n) \times (N - n)$ submatrix of \mathbf{G}_N . Similarly, let \mathbf{y}_n be the n -element subvector of \mathbf{y}_N corresponding to the n in-sample units. Then, under the working regression model (4), and using the in-sample units we compute the weighted least-squares estimate $\hat{\boldsymbol{\theta}}$ of the regression parameter $\boldsymbol{\theta}$:

$$\hat{\boldsymbol{\theta}} = (\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{y}_n,$$

and then predict the unsampled units by $\hat{\mathbf{y}}_{N-n} = \mathbf{Z}_{N-n} \hat{\boldsymbol{\theta}}$.

Under the distribution $F(\cdot)$ and the model including mean difference ψ_N and variance function $g(\cdot)$, the MSE of \hat{T} is $E_{\psi_N, g, F}(\hat{T} - T)^2$. Here, the expectation with respect to the regression model (5) is denoted by $E_{\psi_N, g(\cdot)}$ and the expectation with respect to the distribution $F(\cdot)$ is denoted by $E_F(\cdot)$. We adopt a “minimax” approach in which we choose the sampling design to minimize the MSE, scaled in such a way as to eliminate the dependence on the unknown parameters σ^2 , τ_g^2 , and τ^2 , and maximized over the neighbourhoods of the working distribution and working regression model. In the next section we concentrate on obtaining an upper bound on this maximum scaled mean squared error

$$\mathcal{L}_{\max}^0 = \max_{F \in \mathcal{F}} \max_{g \in \mathcal{G}} \max_{\psi_N \in \Psi} \frac{E_{\psi_N, g, F}(\hat{T} - T)^2}{N [\sigma^2(1 + \tau_g^2) + \tau^2]}. \quad (7)$$

3. MAXIMIZING THE SCALED MEAN SQUARED ERROR

To obtain an upper bound of \mathcal{L}_{\max}^0 , given by (7) we begin by maximizing the MSE over Ψ , and then, we maximize over \mathcal{G} . We finally maximize an upper bound on this second maximum over the neighbourhood \mathcal{F} of the working distribution.

We first require the mean squared error $E_{\psi_N, g, F}(\hat{T} - T)^2$. In the following we employ the definitions, for $h = 1, \dots, L$ and $i, k, l = 1, \dots, N$,

$$D_{h,i}^{k,l} = U_{1hi} + (x_k + x_l)U_{2hi} + x_k x_l U_{3hi},$$

where

$$\begin{aligned} U_{1hi} &= \frac{(B_{2h}x_i - B_{3h})^2}{g_0^2(x_i)D_h^2}, \\ U_{2hi} &= \frac{-(B_{1h}x_i - B_{2h})(B_{2h}x_i - B_{3h})}{g_0^2(x_i)D_h^2}, \\ U_{3hi} &= \frac{(B_{1h}x_i - B_{2h})^2}{g_0^2(x_i)D_h^2}, \end{aligned}$$

and

$$B_{1h} = \sum_{i \in s_h} \frac{1}{g_0(x_i)}, \quad B_{2h} = \sum_{i \in s_h} \frac{x_i}{g_0(x_i)}, \quad B_{3h} = \sum_{i \in s_h} \frac{x_i^2}{g_0(x_i)}, \quad D_h = B_{1h}B_{3h} - B_{2h}^2.$$

Lemma 1 The MSE of \hat{T} with respect to the true regression model (including the mean departure $\psi_N(\cdot)$ and variance function $g(\cdot)$) and true distribution $F(\cdot)$ is given by

$$\begin{aligned} E_{\psi_N, g, F}(\hat{T} - T)^2 &= \sigma^2 \mathbf{1}'_{N-n} \mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h(1 - p_h) \mathbf{R}_{h,g} \right) \mathbf{Q}_r' \mathbf{1}_{N-n} \\ &\quad + \sigma^2 \sum_{k \notin s} g(x_k) + \tau^2 E_F \left(\mathbf{1}'_{N-n} (\mathbf{M}_1 \psi_n - \psi_{N-n}) \right)^2. \end{aligned} \quad (8)$$

Here \mathbf{Q}_r is an $(N - n) \times N$ incidence matrix, with entries 1 or 0 defined by $\mathbf{Z}_{N-n} = \mathbf{Q}_r \mathbf{Z}_N$,

$$\mathbf{M}_1 = \mathbf{Z}_{N-n} (\mathbf{Z}_n' \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}_n' \mathbf{G}_{0,n}^{-1},$$

$\mathbf{C}_{h,g}$ is an $N \times N$ matrix with $(k, l)^{\text{th}}$ entry

$$C_{h,g}^{k,l} = \sum_{i \in s_h} g(x_i) D_{h,i}^{k,l}, \quad (9)$$

and $\mathbf{R}_{h,g} = \text{diag} \left\{ C_{h,g}^{1,1}, \dots, C_{h,g}^{N,N} \right\}$.

Theorem 1 Over Ψ , the MSE of \hat{T} has maximum value

$$\begin{aligned} \max_{\psi_N \in \Psi} E_{\psi_N, g, F}(\hat{T} - T)^2 &= \sigma^2 \mathbf{1}'_{N-n} \mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h(1 - p_h) \mathbf{R}_{h,g} \right) \mathbf{Q}_r' \mathbf{1}_{N-n} \\ &\quad + \sigma^2 \sum_{k \notin s} g(x_k) + \tau^2 ch_{\max} \left(\mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,1} + p_h(1 - p_h) \mathbf{R}_{h,1} \right) \mathbf{Q}_r' \right) + \tau^2. \end{aligned} \quad (10)$$

Here $ch_{\max}(\mathbf{A})$ denotes the maximum eigenvalue of the matrix \mathbf{A} .

We now maximize (10) over $g \in \mathcal{G}$.

Theorem 2 Over \mathcal{G} , $\max_{\psi_N \in \Psi} E_{\psi_N, g, F}(\hat{T} - T)^2$ has maximum value

$$\begin{aligned} \max_{g \in \mathcal{G}} \max_{\psi_N \in \Psi} E_{\psi_N, g, F}(\hat{T} - T)^2 &= \sigma^2(1 + \tau_g^2) \left(\mathbf{p}'_F \mathbf{B} \mathbf{p}_F + \mathbf{c}' \mathbf{p}_F + \sum_{k \notin s} g_0(x_k) \right) \\ &+ \tau^2 c h_{\max} \left(\mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,1} + p_h(1 - p_h) \mathbf{R}_{h,1} \right) \mathbf{Q}'_r \right) + \tau^2. \end{aligned}$$

Here $\mathbf{B} = \text{diag}\{b_h : h = 1, \dots, L\}$ and $\mathbf{c} = (c_1, \dots, c_L)'$, with

$$b_h = \frac{B_{1h} \left(\sum_{k \notin s} x_k \right)^2 - 2B_{2h}(N - n) \sum_{k \notin s} x_k + B_{3h}(N - n)^2}{D_h} - c_h,$$

and

$$c_h = \frac{B_{1h} \sum_{k \notin s} x_k^2 - 2B_{2h} \sum_{k \notin s} x_k + B_{3h}(N - n)}{D_h}.$$

In order to get an upper bound on the maximum value of $\max_{g \in \mathcal{G}} \max_{\psi_N \in \Psi} \frac{E_{\psi_N, g, F}(\hat{T} - T)^2}{\sigma^2(1 + \tau_g^2) + \tau^2}$ over \mathcal{F} we write $\frac{\sigma^2(1 + \tau_g^2)}{\sigma^2(1 + \tau_g^2) + \tau^2} = \gamma$, in terms of which

$$\begin{aligned} \max_{g \in \mathcal{G}} \max_{\psi_N \in \Psi} \frac{E_{\psi_N, g, F}(\hat{T} - T)^2}{\sigma^2(1 + \tau_g^2) + \tau^2} &= \gamma \left(\mathbf{p}'_F \mathbf{B} \mathbf{p}_F + \mathbf{c}' \mathbf{p}_F + \sum_{k \notin s} g_0(x_k) \right) \\ &+ (1 - \gamma) \left(c h_{\max} \left(\mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,1} + p_h(1 - p_h) \mathbf{R}_{h,1} \right) \mathbf{Q}'_r \right) + 1 \right) \\ &\leq \gamma \left(\mathbf{p}'_F \mathbf{B} \mathbf{p}_F + \mathbf{c}' \mathbf{p}_F + \sum_{k \notin s} g_0(x_k) \right) \\ &+ (1 - \gamma) \left(\sum_{h=1}^L p_h^2 c h_{\max}(\mathbf{Q}_r (\mathbf{C}_{h,1}) \mathbf{Q}'_r) + p_h(1 - p_h) c h_{\max}(\mathbf{Q}_r \mathbf{R}_{h,1} \mathbf{Q}'_r) + 1 \right) \\ &= \gamma \left(\mathbf{p}'_F \mathbf{B} \mathbf{p}_F + \mathbf{c}' \mathbf{p}_F + \sum_{k \notin s} g_0(x_k) \right) + (1 - \gamma) \left(\mathbf{p}'_F \mathbf{B}^{ch} \mathbf{p}_F + (\mathbf{c}^{ch})' \mathbf{p}_F + 1 \right) \end{aligned}$$

where $\mathbf{B}^{ch} = \text{diag}\{c h_{\max}(\mathbf{Q}_r \mathbf{C}_{h,1} \mathbf{Q}'_r) - c_h^{ch} : h = 1, \dots, L\}$ and $\mathbf{c}^{ch} = (c_1^{ch}, \dots, c_L^{ch})'$ with $c_h^{ch} = c h_{\max}(\mathbf{Q}_r \mathbf{R}_{h,1} \mathbf{Q}'_r)$. So,

$$\max_{F \in \mathcal{F}} \max_{g \in \mathcal{G}} \frac{E_{\psi_N, g, F}(\hat{T} - T)^2}{\sigma^2(1 + \tau_g^2) + \tau^2} \leq \max_{\mathbf{p}_F \in \mathcal{P}} \left(\mathbf{p}'_F \mathbf{B}_\gamma \mathbf{p}_F + \mathbf{c}'_\gamma \mathbf{p}_F \right) + \gamma \sum_{k \notin s} g_0(x_k) + (1 - \gamma).$$

with $\mathbf{B}_\gamma = \gamma \mathbf{B} + (1 - \gamma) \mathbf{B}^{ch}$, $\mathbf{c}_\gamma = \gamma \mathbf{c} + (1 - \gamma) \mathbf{c}^{ch}$.

TABLE 1: Calculation of \mathcal{L}_{\max} for the samples in Example 1.

Sample (ξ)	(b_1, b_2)	(c_1, c_2)	$\mathcal{L}_{\max}(\xi)$
{0.1, 0.2, 0.6, 0.8}	(7.80, -5.10)	(18.60, 7.50)	4.60
{0.1, 0.2, 0.6, 0.9}	(6.80, -0.40)	(14.30, 3.77)	3.70
{0.1, 0.2, 0.8, 0.9}	(4.80, 46.80)	(7.50, 62.10)	16.70
{0.1, 0.3, 0.6, 0.8}	(0.90, -6.60)	(5.80, 10.55)	1.36
{0.1, 0.3, 0.6, 0.9}	(0.80, -0.67)	(4.40, 5.33)	1.03
{0.1, 0.3, 0.8, 0.9}	(0.60, 51.20)	(2.20, -82.40)	22.40
{0.2, 0.3, 0.6, 0.8}	(-9.00, -8.10)	(23.00, 14.30)	2.71
{0.2, 0.3, 0.6, 0.9}	(-7.60, -1.60)	(16.90, 15.55)	2.57
{0.2, 0.3, 0.8, 0.9}	(-4.80, 63.60)	(7.70, 106.10)	28.40

Following the above analysis we denote

$$\mathcal{L}_{\max} = \mathcal{L}_{\max}(\xi) = \frac{\max_{\mathbf{p}_F \in \mathcal{P}} \left(\mathbf{p}'_F \mathbf{B}_\gamma \mathbf{p}_F + \mathbf{c}'_\gamma \mathbf{p}_F \right) + \gamma \sum_{k \notin s} g_0(x_k) + (1 - \gamma)}{N}$$

as the loss function for a given sampling design ξ . To find this, it suffices to find the maximum value

$$\mathcal{L}_{0,\delta} = \max_{\mathcal{P}} \frac{\mathbf{p}' \mathbf{B}_\gamma \mathbf{p} + \mathbf{c}'_\gamma \mathbf{p}}{N}, \quad (11)$$

since then $\mathcal{L}_{\max} = \mathcal{L}_{0,\delta} + \mathcal{L}_v$, with $\mathcal{L}_v = \gamma \sum_{k \notin s} g_0(x_k) / N + (1 - \gamma) / N$.

Note that there is now no need for the sampler to have available values of σ^2 , τ_g^2 , or τ^2 —he or she need only choose a value of γ , based on his or her relative concern for errors arising from \mathcal{G} rather than from Ψ .

We illustrate Theorem 2 in a simple case ($L = 2$, $\gamma = 1$), in which the calculations are quite transparent and we can easily find the maximum of (11) and of \mathcal{L}_{\max} .

Example 1 Consider a population with $N = 6$ and $x = \{0.1, 0.2, 0.3, 0.6, 0.8, 0.9\}$. Take $L = 2$, stratum sizes $N_1 = N_2 = 3$ with $n = 4$ and $n_1 = n_2 = 2$, and $\gamma = 1$. Assume that $g_0(x) = x$, $\mathbf{p}^0 = (0.5, 0.5)'$, and $\delta = \sqrt{0.5}$. The nine possible samples are enumerated in Table 1; for each of these \mathcal{L}_{\max} is calculated as follows. For the sample $s = \{0.1, 0.3, 0.6, 0.9\}$ we calculate $\mathbf{B}_1 = \text{diag}\{0.8, -0.6667\}$ and $\mathbf{c}_1 = (4.4, 5.3333)'$. We calculate that

$$\mathcal{L}_{0,\delta} = \max_{0 \leq p_2 \leq 1} \frac{0.1333 p_2^2 - 0.6667 p_2 + 5.2}{6} = \frac{5.2}{6},$$

and $\mathcal{L}_v = 1/6$. Thus, $\mathcal{L}_{\max} = 1.0333$ for this (minimax) sample; the other entries of Table 1 are calculated in the same manner.

The next two results give analytic solutions to (11).

Theorem 3 *There exists a solution \mathbf{p}_0 to the problem*

$$\text{maximize } \mathbf{p}'\mathbf{B}_\gamma\mathbf{p} + \mathbf{c}'_\gamma\mathbf{p}, \text{ subject to (i) } \mathbf{1}'\mathbf{p} = 1, \text{ (ii) } \|\mathbf{p} - \mathbf{p}^0\| \leq \delta, \text{ (iii) } \mathbf{p} \succeq \mathbf{0}. \quad (12)$$

This maximizer has elements

$$p_{0,h}(\lambda, \mu) = \left(\frac{\mu p_h^0 + c_h/2 - \lambda}{\mu - b_h} \right)^+,$$

where μ and λ are to maximize

$$\mathbf{p}'\mathbf{B}_\gamma\mathbf{p} + \mathbf{c}'_\gamma\mathbf{p} = \sum_h p_{0,h}(\lambda, \mu) (b_h p_{0,h}(\lambda, \mu) + c_h),$$

subject to (i) and (ii).

If δ is sufficiently small, then Theorem 3 can be made much more explicit.

Theorem 4 *If $\delta \leq \min_h p_h^0$, the maximum value $\mathcal{L}_{0,\delta}$ at (11) can be obtained as follows. Define*

$$\lambda = \lambda(\mu) = \sum_h (b_h p_h^0 + c_h/2) \alpha_h(\mu), \quad (13)$$

for coefficients $\alpha_h(\mu) = (\mu - b_h)^{-1} / \sum_h (\mu - b_h)^{-1}$. Then, the maximizing \mathbf{p}_0 of Theorem 3 has elements

$$p_{0,h}(\lambda, \mu) = \frac{\mu p_h^0 + c_h/2 - \lambda(\mu)}{\mu - b_h}, \quad (14)$$

and

$$\mathcal{L}_{0,\delta} = \max_\mu \frac{\sum_h p_{0,h}(\lambda(\mu), \mu) (b_h p_{0,h}(\lambda(\mu), \mu) + c_h)}{N},$$

with this maximization carried out subject to $\min_h p_{0,h}(\lambda, \mu) \geq 0$ and $\|\mathbf{p}_0 - \mathbf{p}^0\|^2 = \sum_h (p_{0,h}(\lambda(\mu), \mu) - p_h^0)^2 \leq \delta^2$.

Even when $\delta \leq \min_h p_h^0$, Theorems 3 and 4 are inconvenient for numerical work, because they require auxiliary optimizations to be carried out each time a sampling design is assessed. As our numerical algorithm calls for a huge number of such assessments we give another approach. We will solve (12) without the non-negativity requirement (iii), obtaining an explicit maximizer \mathbf{p}_0 in the larger class defined by (i) and (ii). If this \mathbf{p}_0 also satisfies (iii), then it is a fortiori a maximizer in the smaller class \mathcal{P} .

The solution to this problem relies in turn on results for the problem

$$\max_{\|\mathbf{w}\|=\delta} (\mathbf{w}'\mathbf{E}\mathbf{w} + 2\mathbf{d}'\mathbf{w}), \quad (15)$$

for symmetric matrices $\mathbf{E}_{(L-1) \times (L-1)}$. The following Lemma summarizes Lemmas 1 and 2 of Hager (2001).

Lemma 2 (Hager 2001) *The vector \mathbf{w} is a solution vector for (15) if and only if $\|\mathbf{w}\| = \delta$ and there exists μ such that $\mu\mathbf{I} - \mathbf{E}$ is positive semidefinite and $(\mu\mathbf{I} - \mathbf{E})\mathbf{w} = \mathbf{d}$. In terms of the eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{L-1}$ and corresponding orthogonal eigenvectors $\mathbf{w}_1, \dots, \mathbf{w}_{L-1}$ of \mathbf{E} , the vector $\mathbf{w} = \sum_{i=1}^{L-1} c_i \mathbf{w}_i$ is a solution of (15) if and only if \mathbf{c} is chosen in the following way. Define $\Gamma_1 = \{i : \lambda_i = \lambda_1\}$, $\Gamma_2 = \{i : \lambda_i < \lambda_1\}$, and $v_i = \mathbf{d}'\mathbf{w}_i$. Then:*

(i) *If $v_i = 0$ for all $i \in \Gamma_1$ and*

$$\sum_{i \in \Gamma_2} \frac{v_i^2}{(\lambda_i - \lambda_1)^2} \leq \delta^2,$$

then $\mu = \lambda_1$ and $c_i = \frac{v_i}{\lambda_1 - \lambda_i}$ for $i \in \Gamma_2$. The c_i for $i \in \Gamma_1$ can be arbitrarily chosen subject to the condition

$$\sum_{i \in \Gamma_1} c_i^2 = \delta^2 - \sum_{i \in \Gamma_2} \frac{v_i^2}{(\lambda_1 - \lambda_i)^2}.$$

(ii) *If (i) does not apply, then $c_i = \frac{v_i}{\mu - \lambda_i}$, $1 \leq i \leq L-1$, for any $\mu > \lambda_1$ subject to the condition*

$$\sum_{i=1}^{L-1} \frac{v_i^2}{(\lambda_i - \mu)^2} = \delta^2.$$

We can now state the main result, giving the maximized loss $\mathcal{L}_{0,\delta}$ at (11).

Theorem 5 *Denote by \mathcal{P}^0 the class \mathcal{P} defined at (6), without the non-negativity requirement $\mathbf{p} \succeq \mathbf{0}$. Then:*

(i) *The maximizer*

$$\mathbf{p}_0 = \arg \max_{\mathcal{P}^0} \mathbf{p}' \mathbf{B}_\gamma \mathbf{p} + \mathbf{c}'_\gamma \mathbf{p}$$

is given by $\mathbf{p}_0 = \mathbf{p}^0 + \mathbf{D}\mathbf{w}_$, where \mathbf{w}_* is one of (a) the solution of $-\mathbf{E}\mathbf{w} - \mathbf{d} = 0$, or (b) $\sum_{i=1}^{L-1} c_i \mathbf{w}_i$ as in Lemma 2, whichever results in the larger value of $\mathbf{w}_*' \mathbf{E} \mathbf{w}_* + 2\mathbf{d}' \mathbf{w}_*$. Here $\mathbf{E} = \mathbf{D}' \mathbf{B}_\gamma \mathbf{D} : (L-1) \times (L-1)$ and $\mathbf{d} = \mathbf{D}' (\mathbf{B}_\gamma \mathbf{p}^0 + \mathbf{c}_\gamma/2) \in \mathbb{R}^{L-1}$ for an $L \times (L-1)$ matrix \mathbf{D} whose columns form an orthogonal basis of the orthogonal complement to the column space of $\mathbf{1}_L$.*

(ii) *If $\mathbf{p}_0 \succeq \mathbf{0}$ then \mathbf{p}_0 is also the maximizer in \mathcal{P} , and*

$$\mathcal{L}_{0,\delta} = \frac{\mathbf{p}_0' \mathbf{B}_\gamma \mathbf{p}_0 + \mathbf{c}'_\gamma \mathbf{p}_0}{N}.$$

Our algorithm for finding sampling designs which minimize $\mathcal{L}_{0,\delta}$, described in the next section, accepts as candidates only designs for which (ii) of Theorem 5 holds. It often fails if δ is too large, but typically accepts values of δ substantially larger than the upper bound imposed in Theorem 4.

4. COMPUTATIONS AND CASE STUDY

To find a minimax sampling design, minimizing the maximum loss $\mathcal{L}_{\max}(\xi)$ over designs ξ we will use a genetic algorithm. This algorithm samples in each stratum in such a way as to minimize the maximum loss. For some general theory on genetic algorithms, see Mandal et al. (2007). The

algorithm used here is a modification of that of Welsh & Wiens (2013), and so we describe only the general features and differences.

First a “population” of $n_g = 40$ stratified random samples is generated; to construct each of these, we take one random sample in each stratum of pre-specified size $n_h \leq N_h$ and then form a stratified sample $s = \cup_h s_h$ with sample size $n = \sum_h n_h$. This procedure is repeated n_g times, thus yielding the population of sampling designs. A measure of “fitness” is evaluated for each design, with designs having smaller values of \mathcal{L}_{\max} being deemed more fit. Then pairs of “parent” designs are randomly chosen from a probability distribution assigning probabilities to designs which are proportional to their fitness values. Designs chosen to be parents, and the resulting “children,” undergo processes of “crossover” and “mutation.” The major difference between the methods adopted here, and those in Welsh & Wiens (2013), is in the crossover mechanism, by which two parent designs are combined to yield a child. We have introduced a method, which we call “artificial implantation” (AI), to the genetic algorithm. To do AI we identify the best design (i.e., the design with largest fitness value) and its largest stratum. Then we replace the corresponding stratum of each design by that stratum in the best design.

This process is repeated, until the current “generation” of n_g designs has been replaced by n_g new designs. As in Welsh & Wiens (2013), in each generation we identify the $N_{\text{elite}} = n_g \times P_{\text{elite}}$ ($P_{\text{elite}} = 0.05$) most fit designs, which pass through to the next generation unchanged—in effect they become their own children. The effect of this is that the minimum value of \mathcal{L}_{\max} , in each generation, is necessarily non-increasing. The algorithm terminates when it has failed to find an improved design in 200 consecutive generations.

As in Welsh & Wiens (2013) we find that the results are quite insensitive to the choices of tuning constants, mutation probabilities, and other selection parameters. Relative to the crossover method used by them, the AI method results in significantly faster runs, i.e., convergence to an apparent minimum in significantly fewer generations.

We consider the Sugar Farm population (Chambers & Dunstan, 1986) to apply our design methodology in a small but realistic population. This population consists of $N = 338$ sugar cane farms in Queensland, Australia. The population has a single auxiliary variable x representing the area on each farm, ranging from 18 to 280 units, which is assigned to cane planting. This has been scaled via division by the largest farm size to lie in $(0, 1]$. Some possible sources of error, resulting in a misspecified working distribution F_0 , are incorrect self-reporting by landowners and changes in these areas between the time of planting and the time of reporting. Suppose that, based on the auxiliary variable x , the population is divided into $L = 6$ strata with sizes $N_h, h = 1, \dots, L$. Then we form a sample $s = \cup_{h=1}^L s_h$ with sample size $n = 40$ by independently choosing a simple random sample s_h in the h^{th} stratum without replacement. We use proportional allocation to determine the stratum sample size n_h . We use the relative frequencies $\{N_h/N\}_{h=1}^L$ of the strata as the p_h^0 of the strata under $F_0(x)$.

We ran the genetic algorithm described above in the following three cases. In each case we took $\gamma = 0.9$. To see the effect of γ , which determines the size of \mathcal{F} , we also ran the genetic algorithm for Case 2 with $\delta = 0.15$, $g_0(x) = x$ and various values of γ .

Case 1. $N_1 = 79, N_2 = 142, N_3 = 117$.

Here, the strata sample sizes are $n_1 = 9, n_2 = 17, n_3 = 14$, and $\mathbf{p}^0 = (79, 142, 117)' / 338$. To illustrate the need for designs robust against misspecifications of $F_0(x)$ and $g_0(x)$ we first illustrate the effect of δ on the designs. For various values of δ and with $g_0(x) = x$ in (4) we ran the algorithm and found the designs in Figure 1. In all of our design plots, the relative frequencies of the farm sizes used in the designs are plotted against $x \in (0, 1]$. Secondly we illustrate the effect of $g_0(x)$ on designs. When $\delta = 0.15$, the designs for different $g_0(x)$ are listed in Figure 2. These designs tend to become more dispersed as δ increases, less so as the power of x in $g_0(x)$

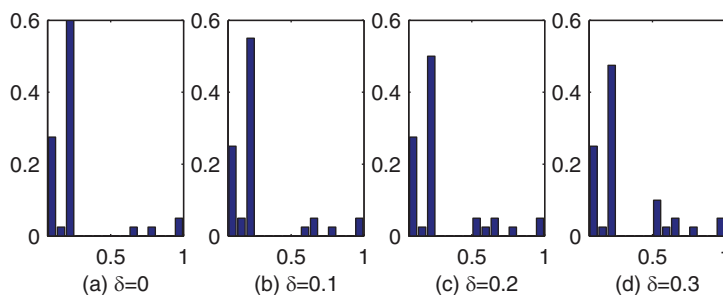


FIGURE 1: Case study; robust designs for Case 1 with $g_0(x) = x$ and varying δ . Relative frequencies of the farm sizes used in the designs vs. scaled farm sizes. [Color figure can be seen in the online version of this article, available at <http://wileyonlinelibrary.com/journal/cjs>]

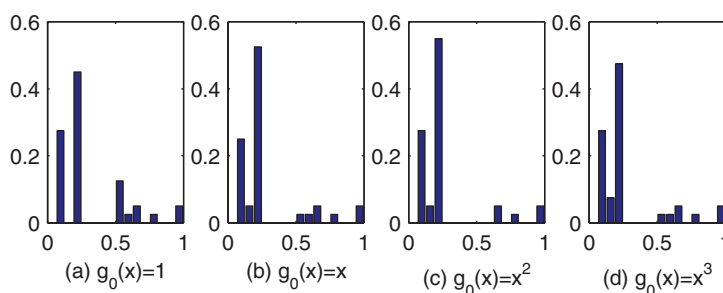


FIGURE 2: Case study; robust designs for Case 1 with $\delta = 0.15$ and varying $g_0(x)$. [Color figure can be seen in the online version of this article, available at <http://wileyonlinelibrary.com/journal/cjs>]

increases. We finally assess the maximum loss in \mathcal{F} to illustrate the difference between the robust and non-robust designs.

When $g_0(x) = x$ and $\delta = 0$ we obtain the design, denoted by ξ_0 , with sampled farm sizes (in the original scale) of

$$x = \left\{ \begin{array}{l} 18, 19, 20, 34(2), 35(6), 36, 59, 60(4), 61(4), 62, 63(3), \\ 64(2), 65, 66(4), 67(3), 68, 186, 213, 263, 280 \end{array} \right\}.$$

This design does not attempt robustness within \mathcal{F} . To assess the protection offered by our minimax designs we calculate the maximum loss $\mathcal{L}_{\max}(\xi_0)$ in \mathcal{F} incurred by ξ_0 at different values of δ . This is compared with the maximum loss $\mathcal{L}_{\max}(\xi_\delta)$ for the design ξ_δ which is minimax for given $\delta > 0$. These comparisons are detailed in Table 2; even for quite small values of δ , the differences are quite significant.

TABLE 2: Case study; maximum losses in \mathcal{F} for robust designs (row 2) and non-robust designs (row 1).

	δ							
	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
$\mathcal{L}_{\max}(\xi_0)$	4.865	5.812	6.915	8.175	9.590	11.161	12.889	14.773
$\mathcal{L}_{\max}(\xi_\delta)$	4.842	5.738	6.742	7.860	9.090	10.422	11.856	13.413

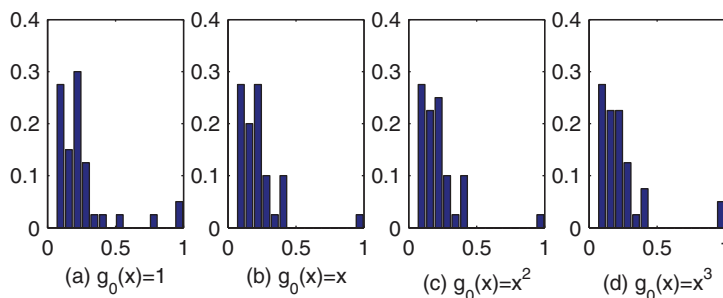


FIGURE 3: Case study; robust designs for Case 2 with $\delta = 0.15$ and varying $g_0(x)$. [Color figure can be seen in the online version of this article, available at <http://wileyonlinelibrary.com/journal/cjs>]

To see the effect of the sampler's choice of distribution $F_0(x)$ we take different $\{N_h\}$ in Case 2 and Case 3.

Case 2. $N_1 = 79$, $N_2 = 54$, $N_3 = 88$, $N_4 = 59$, $N_5 = 31$, $N_6 = 27$.

Here, the strata sample sizes are $n_1 = 9$, $n_2 = 6$, $n_3 = 10$, $n_4 = 7$, $n_5 = 4$, $n_6 = 4$, and $\mathbf{p}^0 = (79, 54, 88, 59, 31, 27)'/338$. We ran the genetic algorithm to find optimal robust designs when $g_0(x) = x$ and $\delta = 0.15$. We found a minimax loss of 19.395 for the robust design (see Figure 3 (b)) with sampled farm sizes of

$$x = \left\{ \begin{array}{l} 18, 19, 20, 34(2), 35(6), 44(3), 45(5), 61, 62, 63(3), \\ 64(2), 65, 66(3), 84(3), 85, 103, 106(3), 110, 280 \end{array} \right\}.$$

The progress of the genetic algorithm is illustrated for one application in Figure 4. We see there that the loss decreases for roughly the first 100 generations and then is fairly stable; the algorithm terminated in fewer than 500 generations.

In Figure 5, designs for a fixed g_0 but different values of δ are presented. Figure 3 shows the effect of $g_0(x)$ on the design. The components of the loss for the optimal design for different values of δ are shown in Table 3 for $g_0(x) = x$, Table 4 for $g_0(x) = x^2$, and Table 5 for $g_0(x) = x^3$.

Case 3. $N_1 = 70$, $N_2 = 63$, $N_3 = 98$, $N_4 = 49$, $N_5 = 28$, $N_6 = 30$.

Here, the strata sample sizes are $n_1 = 8$, $n_2 = 7$, $n_3 = 12$, $n_4 = 6$, $n_5 = 3$, $n_6 = 4$, and $\mathbf{p}^0 = (70, 63, 98, 49, 28, 30)'/338$. We reran the algorithm, with these strata but the remaining inputs as in Case 2, including $\delta = 0.15$ and $g_0(x) = x$, and found a minimax loss of 25.015—

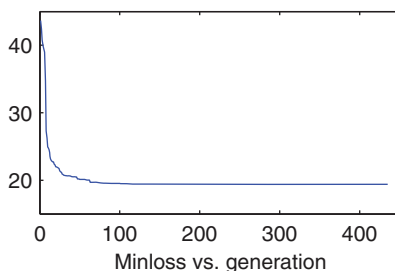


FIGURE 4: Case study; typical progress of the genetic algorithm in one instance of Case 2 using $g_0(x) = x$, $\delta = 0.15$. Minimum loss in each generation is plotted against generation number. [Color figure can be seen in the online version of this article, available at <http://wileyonlinelibrary.com/journal/cjs>]

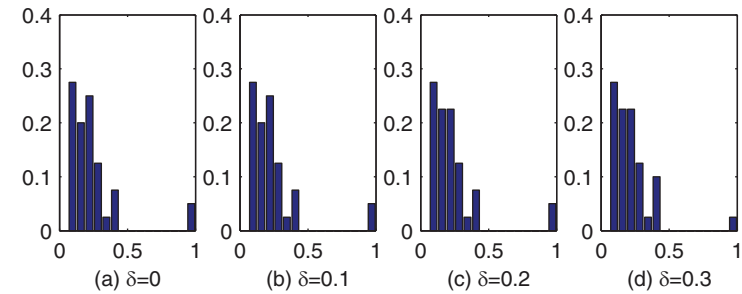


FIGURE 5: Case study; robust designs for Case 2 with $g_0(x) = x^3$ and varying δ . [Color figure can be seen in the online version of this article, available at <http://wileyonlinelibrary.com/journal/cjs>]

TABLE 3: Case study; components of loss for Case 2 with $g_0(x) = x$.

	δ								
	0	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
$\mathcal{L}_{0,\delta}$	9.6482	11.918	15.117	19.225	24.243	30.133	36.917	44.844	53.819
\mathcal{L}_v	0.1682	0.168	0.168	0.170	0.170	0.171	0.171	0.171	0.172
$\mathcal{L}_{\max}(\xi_\delta)$	9.8164	12.086	15.285	19.395	24.413	30.304	37.088	45.015	53.991

TABLE 4: Case study; components of loss for Case 2 with $g_0(x) = x^2$.

	δ								
	0	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
$\mathcal{L}_{0,\delta}$	2.2372	2.9988	4.059	5.438	7.137	9.152	11.438	14.068	17.040
\mathcal{L}_v	0.0465	0.0465	0.046	0.049	0.049	0.050	0.050	0.050	0.050
$\mathcal{L}_{\max}(\xi_\delta)$	2.2837	3.0453	4.105	5.487	7.186	9.202	11.488	14.118	17.090

TABLE 5: Case study; components of loss for Case 2 with $g_0(x) = x^3$.

	δ								
	0	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
$\mathcal{L}_{0,\delta}$	0.829	1.081	1.436	1.901	2.483	3.183	3.979	4.884	5.910
\mathcal{L}_v	0.017	0.017	0.017	0.017	0.017	0.017	0.019	0.019	0.019
$\mathcal{L}_{\max}(\xi_\delta)$	0.846	1.098	1.453	1.918	2.500	3.200	3.998	4.903	5.929

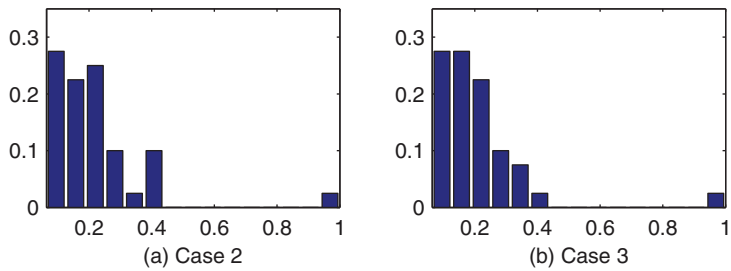


FIGURE 6: Case study; robust designs for Cases 2 and 3 with $g_0(x) = x^2$, $\delta = 0.15$. [Color figure can be seen in the online version of this article, available at <http://wileyonlinelibrary.com/journal/cjs>]

TABLE 6: Case study; components of loss for Case 3 with $g_0(x) = x$.

	δ								
	0	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
$\mathcal{L}_{0,\delta}$	10.706	13.971	18.649	24.844	32.415	41.426	51.843	63.682	77.06
\mathcal{L}_v	0.168	0.170	0.170	0.171	0.172	0.172	0.0172	0.172	0.173
$\mathcal{L}_{\max}(\xi_\delta)$	10.874	14.141	18.819	25.015	32.587	41.598	52.015	63.854	77.233

substantially larger than that in Case 2. The sampled covariates are

$$x = \left\{ \begin{array}{l} 18, 19, 20, 33(2), 34(6), 44(3), 45(7), 66(3), 67(3), \\ 68(3), 69, 84(3), 85, 102(2), 103, 106, 213 \end{array} \right\},$$

which are somewhat different than those in Case 2; in particular the largest farms are not sampled. The effect of this change in \mathbf{p}^0 is illustrated in Figure 6.

The components of the loss for the optimal design for different values of δ are shown in Table 6 for $g_0(x) = x$, Table 7 for $g_0(x) = x^2$, and Table 8 for $g_0(x) = x^3$. Comparing Table 3 with Table 6, Table 4 with Table 7, and Table 5 with Table 8, we observe that, as is to be expected, the minimax loss depends heavily on the initial distribution $F_0(x)$.

We finally wish to check the effect of γ . The components of the loss for the optimal design for different values of γ for Case 2 with $g_0(x) = x$, $\delta = 0.15$ are shown in Table 9. Robust designs for Case 2 with $\gamma = 0.1$ and $\gamma = 0.9$ are illustrated in Figure 7.

TABLE 7: Components of loss for Case 3 with $g_0(x) = x^2$.

	δ								
	0	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
$\mathcal{L}_{0,\delta}$	2.564	3.723	5.409	7.600	10.301	13.463	17.119	21.257	25.865
\mathcal{L}_v	0.047	0.047	0.049	0.049	0.050	0.050	0.051	0.051	0.052
$\mathcal{L}_{\max}(\xi_\delta)$	2.611	3.770	5.458	7.649	10.351	13.513	17.170	21.308	25.917

TABLE 8: Case study; components of loss for Case 3 with $g_0(x) = x^3$.

	δ								
	0	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
$\mathcal{L}_{0,\delta}$	0.953	1.381	2.005	2.828	3.849	5.064	6.442	7.981	9.697
\mathcal{L}_v	0.017	0.017	0.017	0.017	0.017	0.019	0.021	0.021	0.021
$\mathcal{L}_{\max}(\xi_\delta)$	0.970	1.398	2.022	2.845	3.866	5.083	6.463	8.002	9.718

TABLE 9: Case study; components of loss for Case 2 with $g_0(x) = x$, $\delta = 0.15$.

	γ				
	0.1	0.3	0.5	0.7	0.9
$\mathcal{L}_{0,.15}$	5.760	8.679	12.286	15.775	19.225
\mathcal{L}_v	0.021	0.058	0.094	0.132	0.170
$\mathcal{L}_{\max}(\xi_{.15})$	5.782	8.737	12.380	15.907	19.395

5. SUMMARY AND CONCLUSIONS

We have established a method for the construction of sampling designs for model-based stratification that are robust against possible misspecifications of the mean and variance functions in regression models, and the distribution function defining the strata. We obtained an explicit expression for the maximum of the prediction mean squared error for the empirical best predictor over neighbourhoods of the working regression model. It is difficult to find analytically the maximum value of this expression over the neighbourhood of the working distribution function. We therefore chose an upper bound on this maximum value as our loss function. We then implemented a modified genetic algorithm suitable for stratified sampling to find the robust designs which minimize this loss function. We added an “artificial implantation” process into this algorithm to accelerate the speed in searching for the robust design. All these methods are illustrated in a case study of Australian sugar farms. We found that the robust designs did give substantial protection against possible misspecifications of the model and the distribution functions considered in this article.

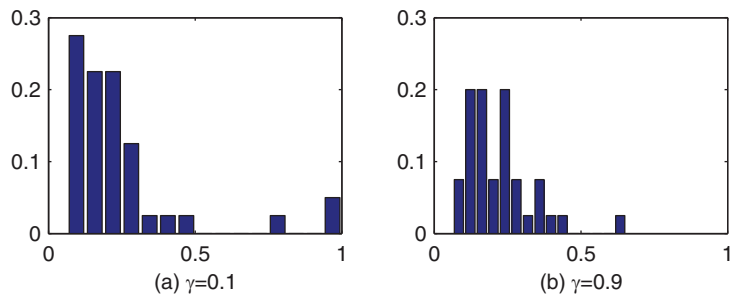


FIGURE 7: Case study; robust designs for Case 2 with $g_0(x) = x$, $\delta = 0.15$ and varying γ . [Color figure can be seen in the online version of this article, available at <http://wileyonlinelibrary.com/journal/cjs>]

APPENDIX

Derivations

Proof of Lemma 1. It follows from $\hat{T} = \sum_{i \in s} Y_i + \sum_{i \notin s} \hat{Y}_i$ that

$$\hat{T} - T = \sum_{i \notin s} (\hat{Y}_i - Y) = \mathbf{1}'_{N-n} (\hat{\mathbf{Y}}_{N-n} - \mathbf{Y}_{N-n}).$$

Under the true model (5),

$$\mathbf{y}_{N-n} = \mathbf{Z}_{N-n} \boldsymbol{\theta} + \boldsymbol{\psi}_{N-n} + \mathbf{G}_{N-n}^{1/2} \boldsymbol{\varepsilon}_{N-n}$$

and $\hat{\mathbf{y}}_{N-n} = \mathbf{Z}_{N-n} \hat{\boldsymbol{\theta}}$; hence

$$\hat{\mathbf{y}}_{N-n} - \mathbf{y}_{N-n} = \mathbf{M} \boldsymbol{\varepsilon}_n - \mathbf{G}_{N-n}^{1/2} \boldsymbol{\varepsilon}_{N-n} + \mathbf{M}_1 \boldsymbol{\psi}_n - \boldsymbol{\psi}_{N-n},$$

where $\mathbf{M} = \mathbf{M}_1 \mathbf{G}_n^{1/2}$. Then

$$\begin{aligned} & (\hat{\mathbf{y}}_{N-n} - \mathbf{y}_{N-n})(\hat{\mathbf{y}}_{N-n} - \mathbf{y}_{N-n})' \\ &= \mathbf{M} \boldsymbol{\varepsilon}_n \boldsymbol{\varepsilon}_n' \mathbf{M}' + \mathbf{G}_{N-n}^{1/2} \boldsymbol{\varepsilon}_{N-n} \boldsymbol{\varepsilon}_{N-n}' \mathbf{G}_{N-n}^{1/2} - \mathbf{M} \boldsymbol{\varepsilon}_n \boldsymbol{\varepsilon}_{N-n}' \mathbf{G}_{N-n}^{1/2} \\ & \quad - \mathbf{G}_{N-n}^{1/2} \boldsymbol{\varepsilon}_{N-n} \boldsymbol{\varepsilon}_n' \mathbf{M}' + (\mathbf{M} \boldsymbol{\varepsilon}_n - \mathbf{G}_{N-n}^{1/2} \boldsymbol{\varepsilon}_{N-n})(\mathbf{M}_1 \boldsymbol{\psi}_n - \boldsymbol{\psi}_{N-n})' \\ & \quad + (\mathbf{M}_1 \boldsymbol{\psi}_n - \boldsymbol{\psi}_{N-n})(\mathbf{M}_1 \boldsymbol{\psi}_n - \boldsymbol{\psi}_{N-n})', \end{aligned}$$

and we find that

$$\begin{aligned} E_{\Psi_{N,g}}(\hat{T} - T)^2 &= \sigma^2 \mathbf{1}'_{N-n} [\mathbf{M} \mathbf{M}' + \mathbf{G}_{N-n}] \mathbf{1}_{N-n} + (\mathbf{1}'_{N-n} (\mathbf{M}_1 \boldsymbol{\psi}_n - \boldsymbol{\psi}_{N-n}))^2 \\ &= \sigma^2 \mathbf{1}'_{N-n} \mathbf{M} \mathbf{M}' \mathbf{1}_{N-n} + \sigma^2 \mathbf{1}'_{N-n} \mathbf{G}_{N-n} \mathbf{1}_{N-n} + (\mathbf{1}'_{N-n} (\mathbf{M}_1 \boldsymbol{\psi}_n - \boldsymbol{\psi}_{N-n}))^2. \end{aligned}$$

With \mathbf{Q}_r as defined in the statement of the Lemma, and noting that $\mathbf{1}'_{N-n} \mathbf{G}_{N-n} \mathbf{1}_{N-n} = \sum_{k \notin s} g(x_k)$ we have

$$E_{\phi_{N,g}}(\hat{T} - T)^2 = \sigma^2 \mathbf{1}'_{N-n} \mathbf{M} \mathbf{M}' \mathbf{1}_{N-n} + \sigma^2 \sum_{k \notin s} g(x_k) + (\mathbf{1}'_{N-n} (\mathbf{M}_1 \boldsymbol{\psi}_n - \boldsymbol{\psi}_{N-n}))^2. \quad (\text{A.1})$$

On the right-hand side of (A.1), only the first and third terms depend on the true distribution function $F(x)$. We only need to calculate the expected values of the first term with respect to $F(x)$. According to the definition of \mathbf{M} we have

$$E_F(\mathbf{1}'_{N-n} \mathbf{M} \mathbf{M}' \mathbf{1}_{N-n}) = E_F \left(\mathbf{1}'_{N-n} \begin{bmatrix} \mathbf{Q}_r \mathbf{Z}_n (\mathbf{Z}_n' \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}_n' \mathbf{G}_{0,n}^{-1} \mathbf{G}_n \\ \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n (\mathbf{Z}_n' \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}_n' \mathbf{Q}_r' \end{bmatrix} \mathbf{1}_{N-n} \right).$$

Note that $\mathbf{Z}_n = (\mathbf{Id}_{s_1}, \mathbf{Id}_{s_1} * \mathbf{x}_n, \dots, \mathbf{Id}_{s_L}, \mathbf{Id}_{s_L} * \mathbf{x}_n)$, with $\mathbf{Id}_{s_h} = (Id_{s_h 1}, \dots, Id_{s_h n})'$ for $Id_{s_h i} = 1$ if $i \in s_h$ and zero otherwise, $h = 1, \dots, L$. Using this we find that

$$\mathbf{Z}_n' \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n = \oplus_{h=1}^L \begin{pmatrix} B_{1h} & B_{2h} \\ B_{2h} & B_{3h} \end{pmatrix},$$

hence

$$(\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} = \oplus_{h=1}^L \left\{ \frac{1}{D_h} \begin{pmatrix} B_{3h} & -B_{2h} \\ -B_{2h} & B_{1h} \end{pmatrix} \right\}.$$

As, in each stratum we take at least two different values of x_i to do regression analysis, the Hölder inequality implies $D_h > 0$. Similarly, with

$$K_{1h} = \sum_{i \in s_h} \frac{g(x_i)}{g_0^2(x_i)}, \quad K_{2h} = \sum_{i \in s_h} \frac{x_i g(x_i)}{g_0^2(x_i)}, \quad K_{3h} = \sum_{i \in s_h} \frac{x_i^2 g(x_i)}{g_0^2(x_i)},$$

we have

$$\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{G}_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n = \oplus_{h=1}^L \begin{pmatrix} K_{1h} & K_{2h} \\ K_{2h} & K_{3h} \end{pmatrix}.$$

After some simplification we obtain

$$(\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{G}_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n (\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} = \oplus_{h=1}^L \begin{pmatrix} W_{1h} & W_{2h} \\ W_{2h} & W_{3h} \end{pmatrix},$$

for

$$W_{1h} = \sum_{i \in s_h} g(x_i) U_{1hi}, \quad W_{2h} = \sum_{i \in s_h} g(x_i) U_{2hi}, \quad W_{3h} = \sum_{i \in s_h} g(x_i) U_{3hi}.$$

It follows that

$$\begin{aligned} & \mathbf{Z}'_N (\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{G}_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n (\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}'_N \\ &= (\mathbf{Id}_1, \mathbf{Id}_1 * \mathbf{x}_N, \dots, \mathbf{Id}_L, \mathbf{Id}_L * \mathbf{x}_N) \left[\oplus_{h=1}^L \begin{pmatrix} W_{1h} & W_{2h} \\ W_{2h} & W_{3h} \end{pmatrix} \right] \mathbf{Z}'_N \\ &= (a_{kl}) \end{aligned}$$

with

$$a_{kl} = \sum_{h=1}^L Id_{hl} Id_{hk} (W_{1h} + (x_k + x_l) W_{2h} + x_l x_k W_{3h}), \text{ for } k, l = 1, \dots, N.$$

The expectation of a_{kl} with respect to $F(\cdot)$ is

$$E_F(a_{kl}) = \begin{cases} \sum_{h=1}^L p_h (W_{1h} + 2x_k W_{2h} + x_k^2 W_{3h}), & k = l, \\ \sum_{h=1}^L p_h^2 (W_{1h} + (x_k + x_l) W_{2h} + x_l x_k W_{3h}), & k \neq l. \end{cases}$$

Thus, with $C_{h,g}^{k,l} = W_{1h} + (x_k + x_l) W_{2h} + x_k x_l W_{3h}$ we obtain

$$\begin{aligned} & E_F[\mathbf{Z}'_N (\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{G}_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n (\mathbf{Z}'_n \mathbf{G}_{0,n}^{-1} \mathbf{Z}_n)^{-1} \mathbf{Z}'_N] \\ &= \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h (1 - p_h) \mathbf{R}_{h,g} \right); \end{aligned}$$

this in (A.1) give us

$$E_F(\mathbf{M}\mathbf{M}') = \sigma^2 \mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h(1-p_h) \mathbf{R}_{h,g} \right) \mathbf{Q}_r'.$$

Here we express $C_{h,g}^{k,l}$ in the simpler and more convenient form (9). ■

Proof of Theorem 1. On the right-hand side of (8), only the term $(\mathbf{1}'_{N-n}(\mathbf{M}_1 \psi_n - \psi_{N-n}))^2$ depends on ψ_N . We must determine its maximum over the set Ψ . Note that

$$\max_{\phi_N \in \Psi} E_F(\mathbf{1}'_{N-n}(\mathbf{M}_1 \psi_n - \psi_{N-n}))^2 = E_F \max_{\phi_N \in \Psi} (\mathbf{1}'_{N-n}(\mathbf{M}_1 \psi_n - \psi_{N-n}))^2.$$

Here

$$\begin{aligned} (\mathbf{1}'_{N-n}(\mathbf{M}_1 \psi_n - \psi_{N-n}))^2 &= (\mathbf{M}_1 \quad -\mathbf{I}) \begin{pmatrix} \psi_n \\ \psi_{N-n} \end{pmatrix} (\psi_n' \quad \psi_{N-n}') \begin{pmatrix} \mathbf{M}_1' \\ -\mathbf{I} \end{pmatrix} \\ &=: \mathbf{M}_0 \phi_N \phi_N' \mathbf{M}_0'. \end{aligned}$$

So

$$\max_{\psi_N \in \Psi} (\mathbf{1}'_{N-n}(\mathbf{M}_1 \psi_n - \psi_{N-n}))^2 = \max_{\psi_N \in \Psi} \|\phi_N' \mathbf{M}_0'\|^2.$$

As ϕ_N can be obtained from ψ_N by reordering, the conditions $\mathbf{Z}'_N \psi_N = 0$ and $\|\psi_N\| \leq \tau$ are equivalent to the existence of $\mathbf{c} \in \mathbb{R}^{N-2L}$ such that $\phi_N = \tau \mathbf{Q} \mathbf{c}$ and $\|\mathbf{c}\| \leq 1$, where columns of \mathbf{Q} form an orthogonal basis for the orthogonal complement to the column space of \mathbf{Z}_N . Thus,

$$\begin{aligned} \max_{\psi_N \in \Psi} \|\phi_N' \mathbf{M}_0'\|^2 &= \max_{\phi_N \in \Psi} (\phi_N' \mathbf{M}_0')^2 = \tau^2 \max_{\|\mathbf{c}\| \leq 1} \mathbf{c}' \mathbf{Q}' \mathbf{M}_0' \mathbf{M}_0 \mathbf{Q} \mathbf{c} \\ &= \tau^2 ch_{\max}(\mathbf{Q}' \mathbf{M}_0' \mathbf{M}_0 \mathbf{Q}) = \tau^2 ch_{\max}(\mathbf{M}_0 \mathbf{M}_0') \\ &= \tau^2 ch_{\max}(\mathbf{M}_1 \mathbf{M}_1' + \mathbf{I}_{N-n}) = \tau^2 \max_{\mathbf{z} \in \mathbb{R}^{N-n}} \mathbf{z}' (\mathbf{M}_1 \mathbf{M}_1') \mathbf{z} + \tau^2; \end{aligned}$$

it follows that

$$E_F \left[\max_{\psi_N \in \Psi} (\mathbf{1}'_{N-n}(\mathbf{M}_1 \psi_n - \psi_{N-n}))^2 \right] = \tau^2 \max_{\mathbf{z} \in \mathbb{R}^{N-n}} \mathbf{z}' [E_F(\mathbf{M}_1 \mathbf{M}_1')] \mathbf{z} + \tau^2.$$

As $\mathbf{M} = \mathbf{M}_1 \mathbf{G}_n^{1/2}$ we have that $\mathbf{M}\mathbf{M}' = \mathbf{M}_1 \mathbf{G}_n \mathbf{M}_1'$. The matrix $\mathbf{M}_1 \mathbf{M}_1'$ can be obtained from $\mathbf{M}\mathbf{M}'$ by taking $\mathbf{G}_n = \mathbf{I}_n$, i.e., $g(x) = 1$. Thus $E_F(\mathbf{M}_1 \mathbf{M}_1') = \mathbf{Q}_r \sum_{h=1}^L [p_h^2 \mathbf{C}_{h,1} + p_h(1-p_h) \mathbf{R}_{h,1}] \mathbf{Q}_r'$, and

$$\begin{aligned} E_F \left[\max_{\phi_N \in \Psi} (\mathbf{1}'_{N-n}(\mathbf{M}_1 \psi_n - \psi_{N-n}))^2 \right] \\ = \tau^2 ch_{\max} \left(\mathbf{Q}_r \sum_{h=1}^L [p_h^2 \mathbf{C}_{h,1} + p_h(1-p_h) \mathbf{R}_{h,1}] \mathbf{Q}_r' \right) + \tau^2. \end{aligned}$$

Here $\mathbf{C}_{h,1} = \mathbf{C}_{h,g}$ with $g = 1$, and $\mathbf{R}_{h,1}$ defined similarly. ■

Proof of Theorem 2. In (10), only the term

$$\mathbf{1}'_{N-n} \mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h(1-p_h) \mathbf{R}_{h,g} \right) \mathbf{Q}'_r \mathbf{1}_{N-n} + \sum_{k \notin s} g(x_k)$$

depends on $g(x)$. Using (9) we obtain

$$\begin{aligned} & \mathbf{1}'_{N-n} \mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h(1-p_h) \mathbf{R}_{h,g} \right) \mathbf{Q}'_r \mathbf{1}_{N-n} + \sum_{k \notin s} g(x_k) \\ &= \sum_{h=1}^L \left(p_h^2 \mathbf{1}'_{N-n} \mathbf{Q}_r \mathbf{C}_{h,g} \mathbf{Q}'_r \mathbf{1}_{N-n} + p_h(1-p_h) \mathbf{1}'_{N-n} \mathbf{Q}_r \mathbf{R}_{h,g} \mathbf{Q}'_r \mathbf{1}_{N-n} \right) + \sum_{k \notin s} g(x_k) \\ &= \sum_{h=1}^L \left(p_h^2 \sum_{k \notin s} \sum_{l \notin s} C_{h,g}^{k,l} + p_h(1-p_h) \sum_{k \notin s} C_{h,g}^{k,k} \right) + \sum_{k \notin s} g(x_k) \\ &= \sum_{h=1}^L \sum_{i \in s_h} g(x_i) \left(p_h^2 \sum_{k \notin s} \sum_{l \notin s} D_{h,i}^{k,l} + p_h(1-p_h) \sum_{k \notin s} D_{h,i}^{k,k} \right) + \sum_{k \notin s} g(x_k) \\ &:= S_{g|s} + S_{g|s^c}. \end{aligned}$$

As $S_{g|s}$ depends only on the value of $g(x)$ in s and $S_{g|s^c}$ depends only on the value of $g(x)$ out of sample s ,

$$\begin{aligned} & \max_{g \in \mathcal{G}} \left(\mathbf{1}'_{N-n} \mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h(1-p_h) \mathbf{R}_{h,g} \right) \mathbf{Q}'_r \mathbf{1}_{N-n} + \sum_{k \notin s} g(x_k) \right) \\ &= \max_{g \in \mathcal{G}} S_{g|s} + \max_{g \in \mathcal{G}} S_{g|s^c}. \end{aligned}$$

For the maximum problem out of sample s we have

$$\max_{g \in \mathcal{G}} S_{g|s^c} = \max_{g \in \mathcal{G}} \sum_{k \notin s} g(x_k) = (1 + \tau_g^2) \sum_{k \notin s} g_0(x_k), \quad (\text{A.2})$$

attained with $g(x_k) = (1 + \tau_g^2)g_0(x_k)$ for all $k \notin s$.

It remains to solve the maximization problem in sample s . Note that $U_{2hi} = -\sqrt{U_{1hi}U_{3hi}}$, so that

$$D_{h,i}^{k,k} = U_{3hi}x_k^2 + 2U_{2hi}x_k + U_{1hi} = \left(x_k \sqrt{U_{3hi}} - \sqrt{U_{1hi}} \right)^2 \geq 0,$$

hence

$$\sum_{k \notin s} D_{h,i}^{k,k} \geq 0. \quad (\text{A.3})$$

Similarly,

$$\sum_{k \notin s} \sum_{l \notin s} D_{h,i}^{k,l} = U_{3hi} \left(\sum_{k \notin s} x_k \right)^2 + 2(N-n)U_{2hi} \left(\sum_{k \notin s} x_k \right) + (N-n)^2 U_{1hi} \geq 0. \quad (\text{A.4})$$

Note also that $p_h(1 - p_h) \geq 0$ for all h . Then, using (A.3) and (A.4) we have

$$\begin{aligned} \max_{g \in \mathcal{G}} S_{g|s} &= \max_{g \in \mathcal{G}} \left(\sum_{h=1}^L \sum_{i \in s_h} g(x_i) \left(p_h^2 \sum_{k \notin s} \sum_{l \notin s} D_{h,i}^{k,j} + p_h(1 - p_h) \sum_{k \notin s} D_{h,i}^{k,k} \right) \right) \\ &= (1 + \tau_g^2) \sum_{h=1}^L \sum_{i \in s_h} g_0(x_i) \left(p_h^2 \sum_{k \notin s} \sum_{l \notin s} D_{h,i}^{k,j} + p_h(1 - p_h) \sum_{k \notin s} D_{h,i}^{k,k} \right) \quad (\text{A.5}) \end{aligned}$$

by taking $g(x_i) = (1 + \tau_g^2)g_0(x_i)$ for all $i \in s$.

Combining (A.2) and (A.5) we obtain, after a rearrangement,

$$\begin{aligned} \max_{g \in \mathcal{G}} &\left(\mathbf{1}'_{N-n} \mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h(1 - p_h) \mathbf{R}_{h,g} \right) \mathbf{Q}'_r \mathbf{1}_{N-n} + \sum_{k \notin s} g(x_k) \right) \\ &= (1 + \tau_g^2) \left[\sum_{h=1}^L \left(p_h^2 \left(\sum_{k \notin s} \sum_{l \notin s} C_{h,g_0}^{k,l} - \sum_{k \notin s} C_{h,g_0}^{k,k} \right) + p_h \sum_{k \notin s} C_{h,g_0}^{k,k} \right) + \sum_{k \notin s} g_0(x_k) \right]. \end{aligned}$$

Finally, upon inserting $C_{h,g_0}^{k,l} = (B_{3h} - (x_k + x_l)B_{2h} + x_k x_l B_{1h}) / D_h$,

$$\begin{aligned} \max_{g \in \mathcal{G}} &\left(\mathbf{1}'_{N-n} \mathbf{Q}_r \sum_{h=1}^L \left(p_h^2 \mathbf{C}_{h,g} + p_h(1 - p_h) \mathbf{R}_{h,g} \right) \mathbf{Q}'_r \mathbf{1}_{N-n} + \sum_{k \notin s} g(x_k) \right) \\ &= (1 + \tau_g^2) \left(\mathbf{p}'_F \mathbf{B} \mathbf{p}_F + \mathbf{c}'_F \mathbf{p}_F + \sum_{k \notin s} g_0(x_k) \right), \end{aligned}$$

with \mathbf{B} and \mathbf{c} as in the statement of the Theorem. ■

Proof of Theorem 3. Write the constraint (ii) as

$$(\text{ii})': \delta^2 - \beta^2 - \|\mathbf{p} - \mathbf{p}^0\|^2 = 0, \text{ for a slack variable } \beta^2.$$

Denote by \mathbf{p}_0 the maximizer, which is guaranteed to exist as the objective function is continuous on its compact domain. Let $\mathbf{p}_1 \in \mathcal{P}$ be arbitrary, define $\mathbf{p}_t = (1 - t)\mathbf{p}_0 + t\mathbf{p}_1$, ($0 \leq t \leq 1$) and consider the function

$$\Phi(t; \mu, \lambda) = \frac{\mathbf{p}'_t \mathbf{B}_\gamma \mathbf{p}_t + \mathbf{c}'_\gamma \mathbf{p}_t - 2\lambda (\mathbf{1}' \mathbf{p}_t - 1) + \mu (\delta^2 - \beta^2 - \|\mathbf{p}_t - \mathbf{p}^0\|^2)}{N}.$$

In order that \mathbf{p}_0 be the maximizer, it is necessary and sufficient that $\Phi(t, \mu, \lambda)$ be maximized at $t = 0$ for all \mathbf{p}_1 , for multipliers λ and μ chosen to satisfy the side conditions (i) and (ii)'. This condition is that, for all \mathbf{p}_1 ,

$$0 \geq \Phi'(0; \mu, \lambda) = \frac{(-2(\mu \mathbf{I} - \mathbf{B}_\gamma) \mathbf{p}_0 + \mathbf{c}_\gamma - 2\lambda \mathbf{1} + 2\mu \mathbf{p}^0)' (\mathbf{p}_1 - \mathbf{p}_0)}{N}. \quad (\text{A.6})$$

Condition (A.6) entails

$$\begin{aligned} \left(-2 (\mu \mathbf{I} - \mathbf{B}_\gamma) \mathbf{p}_0 + \mathbf{c}_\gamma - 2\lambda \mathbf{1} + 2\mu \mathbf{p}^0 \right)_h &= 0 \text{ if } \mathbf{p}_{0,h} > 0, \\ \left(-2 (\mu \mathbf{I} - \mathbf{B}_\gamma) \mathbf{p}_0 + \mathbf{c}_\gamma - 2\lambda \mathbf{1} + 2\mu \mathbf{p}^0 \right)_h &\leq 0 \text{ if } \mathbf{p}_{0,h} = 0; \end{aligned}$$

i.e.,

$$p_{0,h}(\lambda, \mu) = \left(\frac{\mu \mathbf{p}_h^0 + \mathbf{c}_h/2 - \lambda}{\mu - b_h} \right)^+,$$

with λ and μ determined by (i) and (ii)', and with β^2 then chosen to maximize the objective function. Equivalently, λ and μ are determined by the requirement that they maximize the objective function, subject to (i) and (ii). ■

Proof of Theorem 4. If $\delta \leq \min_h p_h^0$ then $\mathbf{p} \succsim \mathbf{0}$ for all \mathbf{p} for which $\|\mathbf{p} - \mathbf{p}^0\| \leq \delta$; in particular the solution given by Theorem 3 satisfies (14), with λ determined by (13) in order to satisfy constraint (i). ■

Proof of Theorem 5. (i) Set $\mathbf{v} = \mathbf{p} - \mathbf{p}^0$. Then

$$\max_{\mathbf{p}^0} \mathbf{p}' \mathbf{B}_\gamma \mathbf{p} + \mathbf{c}'_\gamma \mathbf{p} = \mathcal{L}_0 + \mathcal{L}_\delta^0, \quad (\text{A.7})$$

where

$$\begin{aligned} \mathcal{L}_0 &= \left(\mathbf{p}^0 \right)' \mathbf{B}_\gamma \mathbf{p}^0 + \mathbf{c}'_\gamma \mathbf{p}^0, \text{ and} \\ \mathcal{L}_\delta^0 &= \max_{\mathbf{v}: \mathbf{1}'_L \mathbf{v} = 0, \|\mathbf{v}\| \leq \delta} \mathbf{v}' \mathbf{B}_\gamma \mathbf{v} + (2\mathbf{B}_\gamma \mathbf{p}^0 + \mathbf{c}_\gamma)' \mathbf{v}. \end{aligned}$$

Thus, it suffices to find \mathcal{L}_δ^0 . The orthogonality condition $\mathbf{1}'_L \mathbf{v} = 0$ holds if and only if \mathbf{v} lies in the orthogonal complement to the column space of $\mathbf{1}_L$. Denote by \mathbf{D} the $L \times (L-1)$ matrix whose columns form an orthogonal basis for this orthogonal complement. Then, $\mathbf{v} = \mathbf{D}\mathbf{w}$ for some $\mathbf{w} \in \mathbb{R}^{L-1}$ with $\|\mathbf{w}\| = \|\mathbf{v}\| \leq \delta$, and

$$\mathcal{L}_\delta^0 = \max_{\|\mathbf{w}\| \leq \delta} \mathbf{w}' \mathbf{E} \mathbf{w} + 2\mathbf{d}' \mathbf{w}, \quad (\text{A.8})$$

with $\mathbf{E} = \mathbf{D}' \mathbf{B}_\gamma \mathbf{D} : (L-1) \times (L-1)$ and $\mathbf{d} = \mathbf{D}' (\mathbf{B}_\gamma \mathbf{p}^0 + \mathbf{c}_\gamma/2) \in \mathbb{R}^{L-1}$. If \mathbf{w}_* is a solution to Problem (A.8), then

$$\mathbf{p}_0 = \mathbf{p}^0 + \mathbf{D}\mathbf{w}_*$$

is a solution to Problem (A.7).

Problem (A.8) is a quadratic optimization problem over a closed ball. The optimizer is either in the interior or on the boundary of the ball. We claim that the maximizer in (A.8) is either the solution to $-\mathbf{E}\mathbf{w} - \mathbf{d} = 0$ or the solution to (15). For this we consider the following three possibilities:

Case 1: \mathbf{E} is positive semidefinite. In this case (A.8) is a problem of maximizing a convex function over a convex set. According to Corollary 32.3.2 of Rockafellar (1970), the solution of (A.8) must be a boundary point of $\|\mathbf{w}\| \leq \delta$. Thus, it suffices to solve (15).

Case 2: \mathbf{E} is negative semidefinite. If the maximizer \mathbf{w} of (A.8) is obtained in the interior of $\|\mathbf{w}\| \leq \delta$, then the problem

$$\min_{\|\mathbf{w}\| \leq \delta} \mathbf{w}'(-\mathbf{E})\mathbf{w} - 2\mathbf{d}'\mathbf{w}$$

has a solution in the interior of $\|\mathbf{w}\| \leq \delta$. It must be the global minimizer as $-\mathbf{E}$ is positive semidefinite. So, the minimizer is the solution to $-\mathbf{E}\mathbf{w} - \mathbf{d} = 0$.

Case 3: \mathbf{E} is neither positive semidefinite nor negative semidefinite. According to Lemma 2.4 of Sorensen (1982), the maximizer \mathbf{w} of (A.8) is a solution to the equation

$$(\lambda \mathbf{I} - \mathbf{E})\mathbf{w} = \mathbf{d}$$

with $\lambda \geq 0$, $\lambda(\|\mathbf{w}\|^2 - \delta^2) = 0$, and $\lambda \mathbf{I} - \mathbf{E}$ positive semidefinite. As \mathbf{E} is not positive semidefinite or negative semidefinite, the largest eigenvalue λ_1 of \mathbf{E} must be positive. Thus, choose $\lambda \geq \lambda_1 > 0$ so that $\lambda \mathbf{I} - \mathbf{E}$ is positive semidefinite. Then, $\lambda(\|\mathbf{w}\|^2 - \delta^2) = 0$ implies that the maximizer \mathbf{w} must satisfy $\|\mathbf{w}\| = \delta$.

This establishes our claim, and completes the proof of (i). Assertion (ii) is immediate. ■

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