ROBUST MODEL-BASED STRATIFIED SAMPLING DESIGNS

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Abstract We study robust sampling designs for model-based stratification, when the assumed distribution $F_0(\cdot)$ of an auxiliary variable x, and the variance function $g_0(\cdot)$ in the associated regression model, are only approximately specified. We first maximize the scaled prediction mean squared error (SPMSE) for the empirical best predictor over the neighbourhoods of F_0 and g_0. Then we obtain robust sampling designs which minimize this maximum SPMSE 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, given the farm sizes.

Key words and phrases Artificial implantation; Genetic algorithm; Minimax; Non-informative sampling; Optimal design; Prediction; Stratification

1 Introduction

Due to their nonhomogeneity, populations such as are 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 $\mathbf{x}_1, \ldots, \mathbf{x}_N$. From each of L strata a sample s_h, of pre-specified size $n_h \leq N_h$ (= the population size in the h^{th} stratum), is drawn independently. 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*.

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Since 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 the following model in the h^{th} stratum:

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

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 $T^{EB} = \sum_h N_h \overline{y}_{n_h}$. Here $\overline{y}_{n_h}$ 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 $\hat{\sigma}_{n_h}^2 = \frac{1}{n_h}\sum_{i \in s_h}(y_i - \overline{y}_{n_h})^2$ is the unbiased estimator of the variance σ_h^2 of Y-values in the h^{th} strata.

In the sample 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 $b_1, b_2, \ldots b_{L-1}$ of the target variable Y based on an 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 with density function $f(\cdot)$ when estimating the mean of 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:

$$0 = a_1 < a_2 < \ldots < a_h < \ldots < a_{L-1} < a_L = 1,$$

then

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

Such points $a_1, \ldots, a_L$ will be chosen to minimize the prediction mean square error of an estimator for a population parameter, such as the population total T_y. Since the equations derived by Dalenius are generally unsolvable, Dalenius and Hodges (1959) derived method to find approximately optimum boundaries. See Horgan (2006) for more methods of constructing stratum boundaries, and Ghosh (1963) for optimum stratification with bivariate predictors.

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. For example, assume the following model is valid for all the units in the population:

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

Here $g_0(x) > 0$, and $\varepsilon_1, \ldots, \varepsilon_N$ ($N = \sum_{h=1}^{L} N_h$) are independent and identically distributed random variables with mean zero and variance σ^2. 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 $x_1, \ldots, x_N$ to estimate or predict the finite population total $T = \sum_{i=1}^{N} Y_i$. The *design problem* is to specify a rule using $x_1, \ldots, x_N$ to select a sample s so that the estimator/predictor $\hat{T}$ is a member of class of 'acceptable' estimators/predictors of T, and $\hat{T}$ is optimal in that it minimizes a loss function such as the mean squared error (MSE) $E(T - \hat{T})^2$.

In these methods of modelling heterogeneity, the distribution $F_0(\cdot)$ and the assumed variance function $g_0(\cdot)$ will typically only approximate reality, at best. It is perhaps more realistic to assume only that $F_0(\cdot)$ and $g_0(\cdot)$ are good approximations – we shall refer to them as a working distribution and a working variance function respectively – without necessarily being exact; we then construct robust sampling designs which give good results both at and 'near' this working distribution and this working variance function.

Welsh and Wiens (2013) developed robust, model-based designs for a general class of models which includes the ratio model as a special case. Here we 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 and Wiens (2000), who constructed designs to minimize the (maximized) mean square predicted error; also Dette and Wong (1996) and Wiens and Xu (2008), who studied robustness properties of optimal extrapolation designs. Some general remarks on model-based design strategies are given by Nedyalkova and Tillé (2008). A survey of robustness of design is in Wiens (2014).

In §2 of this article we define explicitly the neighbourhoods of the working distribution and working variance function. In §3 we calculate the MSE for the empirical best predictor under the true distribution $F(\cdot)$ and the true variance function $g(\cdot)$. We then maximize this MSE over a neighbourhood of the working variance function $g_0(\cdot)$. We find that the resulting maximum is a quadratic function of the probabilities of strata under the true distribution function, and go on to maximize over a neighbourhood of the working distribution $F_0(\cdot)$. In this way we obtain the maximized loss function, to be minimized over the class of possible sampling designs. This minimization is a complex numerical problem which we handle, in §4, via a genetic algorithm. We introduce a novel process of 'artificial implantation' into this algorithm – this greatly accelerates its progress – and go on to find the optimal design for the Sugar Farm population (Chambers and Dunstan 1986).

All derivations are in the appendix.

2 The neighbourhoods of the working distribution and working variance function

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

$$\mathbf{y}_N = \mathbf{Z}_N \boldsymbol{\theta} + \mathbf{G}_{0,N}^{1/2} \boldsymbol{\varepsilon}_N, \tag{3}$$

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

Suppose that the true distribution of x is $F(\cdot)$, but that the experimenter mistakenly adopts 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 $\mathbf{p}_F := (p_{F,1}, \ldots, p_{F,L})'$ we define the neighbourhood of the working distribution $F_0(\cdot)$ to be

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

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

$$\mathcal{P} = \{\mathbf{p} \mid \left\|\mathbf{p} - \mathbf{p}^0\right\| \leq \delta; \mathbf{p} \succsim \mathbf{0}, \mathbf{1}_L'\mathbf{p} = 1\}, \tag{4}$$

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, instead of the working variance function $g_0(\cdot)$, the true variance function is $g(\cdot) > 0$ '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. Then, instead of the working model (3), the true model is now

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

where $\mathbf{G}_N = \mathrm{diag}\{g(x_1), \ldots, g(x_N)\}$.

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 $E(Y_i | Y_j, j \in s, x_1, \ldots, x_N)$. Under the working model (3), 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 $\mathbf{G}_{0,n}$ and $\mathbf{G}_{n,N-n}$ to be the $n \times n$ and $(N-n) \times (N-n)$ submatrices 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 model (3), 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 true distribution $F(\cdot)$ and the true variance function $g(\cdot)$, the MSE of $\hat{T}$ is $E_{g,F}(\hat{T}-T)^2$. Here, the expectation with respect to true model (5) with variance function $g(\cdot)$ is denoted by $E_g(\cdot)$ and the expectation with respect to the true 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 and τ_g^2, and maximized over the neighbourhoods of the working distribution and working variance function. In the next section we concentrate on obtaining this maximum scaled mean squared error

$$\mathcal{L}_{\max} = \max_{F \in \mathcal{F}} \max_{g \in \mathcal{G}} \frac{E_{g,F}(\hat{T}-T)^2}{N\sigma^2(1+\tau_g^2)}. \tag{6}$$

3 Maximizing the scaled mean squared error

We will study the optimization problem of obtaining $\mathcal{L}_{\max}$, given by (6). We begin with the first stage maximization over the neighbourhood of the working variance function. Then, we maximize this first stage maximum over the neighbourhood of the working distribution.

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

$$\begin{aligned} D_{h,i}^{k,l} &= U_{1hi} + (x_k + x_l) U_{2hi} + x_k x_l U_{3hi}, \\ D_h &= B_{1h} B_{3h} - B_{2h}^2, \end{aligned}$$

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

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

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

$$\frac{E_{g,F}(\hat{T} - T)^2}{\sigma^2} = \mathbf{1}'_{N-n}\mathbf{Q}_r \sum_{h=1}^{L} \left(p_h^2 \mathbf{C}_{h,g} + p_h(1-p_h)\mathbf{R}_{h,g}\right) \mathbf{Q}'_r \mathbf{1}_{N-n} + \sum_{k \notin s} g\left(x_k\right). \tag{7}$$

Here $\mathbf{Q}_r$ *is an* $(N-n) \times N$ *incidence matrix, with entries* 1 *or* 0 *defined by* $\mathbf{Z}_{N-n} = \mathbf{Q}_r \mathbf{Z}_N$, $\mathbf{C}_{h,g}$ *is an* $N \times N$ *matrix with* $(k,l)^{th}$ *entry*

$$C_{h,g}^{k,l} = \sum_{i \notin s_h} g(x_i) D_{h,i}^{k,l}, \tag{8}$$

and $\mathbf{R}_{h,g} = \oplus_{k=1}^{N} C_{h,g}^{k,k}$.

We now maximize (7) over $g \in \mathcal{G}$.

Theorem 1 *The* MSE $E_{g,F}(\hat{T} - T)^2$ *satisfies*

$$\max_{g \in \mathcal{G}} \frac{E_{g,F}(\hat{T} - T)^2}{N\sigma^2(1+\tau_g^2)} = \frac{\mathbf{p}'_F \mathbf{B} \mathbf{p}_F + \mathbf{c}'\mathbf{p}_F + \sum_{k \notin s} g_0\left(x_k\right)}{N}. \tag{9}$$

Here $\mathbf{B} = \mathrm{diag}\{b_h : h = 1, \ldots, L\}$ *and* $\mathbf{c} = (c_1, .., c_L)'$, *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

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

Following Theorem 1 we continue the development by maximizing (9) over the neighbourhood $\mathcal{F}$ of $F_0(\cdot)$. For this it suffices to find the maximum value

$$\mathcal{L}_{0,\delta} = \max_{\mathcal{P}} \frac{\mathbf{p}'\mathbf{B}\mathbf{p} + \mathbf{c}'\mathbf{p}}{N}, \tag{10}$$

since then

$$\mathcal{L}_{\max} = \mathcal{L}_{0,\delta} + \mathcal{L}_v$$

with $\mathcal{L}_v = \sum_{k \notin s} g_0\left(x_k\right)/N$.

Theorem 2 *There exists a solution* $\mathbf{p}_0$ *to the problem*

$$\text{maximize } \mathbf{p}'\mathbf{B}\mathbf{p} + \mathbf{c}'\mathbf{p}, \text{ subject to (i) } \mathbf{1}'\mathbf{p} = 1, \text{ (ii) } \left\| \mathbf{p} - \mathbf{p}^0 \right\| \leq \delta, \text{ (iii) } \mathbf{p} \gtrsim \mathbf{0}. \tag{11}$$

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*

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

subject to (i) and (ii).

If δ is sufficiently small, then Lemma 2 can be made much more explicit.

Theorem 3 *If* $\delta \leq \min_h p_h^0$, *the maximum value* $\mathcal{L}_{0,\delta}$ *at (10) can be obtained as follows. Define*

$$\lambda = \lambda(\mu) = \sum_h (b_h p_h^0 + c_h/2)\alpha_h(\mu), \tag{12}$$

for coefficients $\alpha_h(\mu) = (\mu - b_h)^{-1} / \sum_h (\mu - b_h)^{-1}$. *Then the maximizing* $\mathbf{p}_0$ *of Lemma 2 has elements*

$$p_{0,h}(\lambda, \mu) = \frac{\mu p_h^0 + c_h/2 - \lambda(\mu)}{\mu - b_h}, \tag{13}$$

and

$$\mathcal{L}_{0,\delta} = \max_\mu \frac{\sum_h p_{0,h}(\lambda(\mu), \mu)\left(b_h p_{0,h}(\lambda(\mu), \mu) + c_h \right)}{N}, \tag{14}$$

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

Even when $\delta \leq \min_h p_h^0$, Theorems 2 and 3 are inconvenient for numerical work, since they requires auxiliary optimizations to be carried out each time a sampling design is assessed. Since our numerical algorithm calls for a huge number of such assessments, we give another approach. We will solve (11) 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

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

with 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* $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{L-1}$ *and corresponding orthogonal eigenvectors* $\mathbf{w}_1, \cdots, \mathbf{w}_{L-1}$ *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* $\nu_i = \mathbf{d}'\mathbf{w}_i$. *Then:*

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

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

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

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

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

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

We can now state the main result, giving the maximized loss $\mathcal{L}_{0,\delta}$ at (10).

Theorem 4 *Denote by* $\mathcal{P}^0$ *the class* $\mathcal{P}$ *defined at (4), without the non-negativity requirement* $\mathbf{p} \succsim \mathbf{0}$. *Then:*

(i) The maximizer

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

is given by $\mathbf{p}_0 = \mathbf{p}^0 + \mathbf{D}\mathbf{w}_*$, *where* $\mathbf{w}_*$ *is one of (a)* $-\mathbf{E}^{-1}\mathbf{d}$, *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* $\mathbf{E} = \mathbf{D}'\mathbf{B}\mathbf{D} : (L-1) \times (L-1)$ *and* $\mathbf{d} = \mathbf{D}'(\mathbf{B}\mathbf{p}^0 + \mathbf{c}/2) \in \mathbb{R}^{L-1}$ *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 $\mathbf{p}_0 \succsim \mathbf{0}$ *then* $\mathbf{p}_0$ *is also the maximizer in* $\mathcal{P}$, *and*

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

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 4 holds. It often fails if δ is too large, but typically accepts values of δ substantially larger than the upper bound imposed in Theorem 3.

4 Minimizing the loss function for the sugar farm population

We will use a genetic algorithm to find the optimal robust design, which samples in each strata in such a way as to minimizes the loss $\mathcal{L}_{\max}$ given in the preceding section. For some general theory on genetic algorithms, see Mandal, Johnson, Wu and Bornemeier (2007). The algorithm used here is a modification of that of Welsh and Wiens (2013), and so we describe only the general features and differences.

First a 'population' of n_g 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 and Wiens (2013), are 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 level) 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 and Wiens (2013), in each generation we identity the $N_{elite} = n_g \times P_{elite}$ 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 nonincreasing. The algorithm terminates when it has failed to find an improved design in 200 consecutive generations. We have used $n_g = 40$ and $P_{elite} = .05$, but find that the results are quite insensitive to these and other tuning constants. Relative to the crossover method used in Welsh and Wiens (2013), the AI method does result in significantly faster runs, i.e. convergence to an apparent minimum in significantly fewer generations.

We consider the sugar farm population (Chambers and Dunstan 1986) to

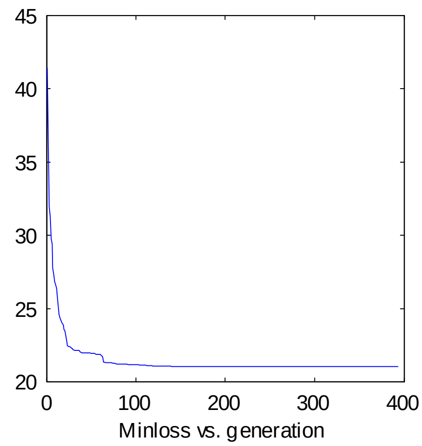

Figure 1: Case 1, $g_0(x) = x, \delta = 0.15$

Table 1. Sugar farm: components of loss for Case 1, $g_0(x) = x$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$\mathcal{L}_{0,\delta}$	10.299	12.816	16.336	20.851	26.394	32.890	40.403	49.131	59.050
$\mathcal{L}_v$	0.186	0.186	0.188	0.188	0.188	0.190	0.190	0.190	0.190
$\mathcal{L}_{\max}$	10.485	13.002	16.524	21.039	26.582	33.080	40.593	49.321	59.240

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 which is the area on each farm assigned to cane planting. Assume that, based on the auxiliary variable x, the population is divided into six strata $(L = 6)$ with sizes $N_h, h = 1, \ldots, L$. 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 strata sample size n_h. We use the relative frequencies $\{N_h/N\}_{h=1}^{L}$ of the six strata as the p_h^0 of the strata under the working distribution $F_0(x)$.

We ran the genetic algorithm described above in the following two cases.

Table 2. Sugar farm: components of loss for Case 1, $g_0(x) = x^2$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$L_{0,\delta}$	2.118	2.939	4.100	5.619	7.489	9.665	12.178	15.024	18.258
L_v	0.051	0.053	0.054	0.054	0.054	0.055	0.056	0.056	0.056
$\mathcal{L}_{\max}$	2.169	2.992	4.154	5.673	7.543	9.720	12.234	15.080	18.314

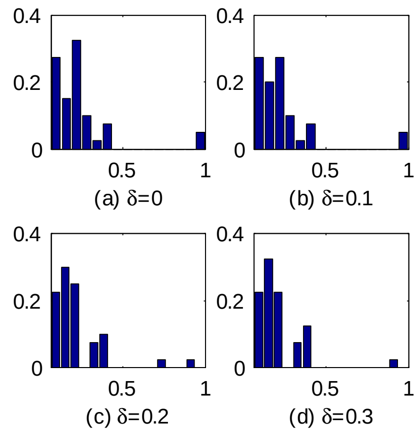

Figure 2: Robust designs for case 1 with $g_0(x) = x^3$

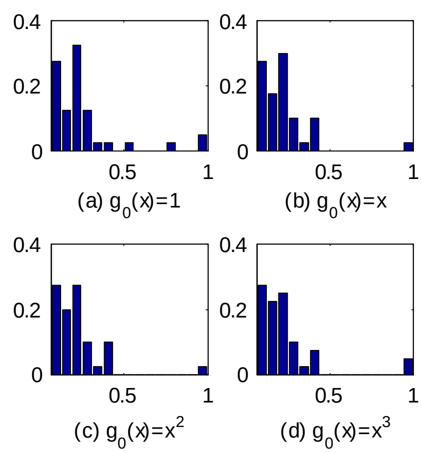

Figure 3: Robust designs for Case 1 with $\delta = 0.15$

Table 3. Sugar farm: components of loss for Case 1, $g_0(x) = x^3$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$\mathcal{L}_{0,\delta}$	0.577	0.873	1.275	1.785	2.400	3.121	3.924	4.845	5.896
$\mathcal{L}_v$	0.018	0.018	0.018	0.018	0.020	0.021	0.021	0.022	0.021
$\mathcal{L}_{\max}$	0.595	0.891	1.293	1.803	2.421	3.142	3.945	4.866	5.917

Case 1. $N_1 = 79$, $N_2 = 54$, $N_3 = 88$, $N_4 = 59$, $N_5 = 31$, $N_6 = 27$.

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 $\mathbf{p}^0 = (79/338, 54/338, 88/338, 59/338, 31/338, 27/338)'$. We ran the algorithm to find optimal robust designs for the working distribution and variance function in (3) with $g_0(x) = x$ and $\delta = 0.15$. We found a minimum loss of 21.039. For the robust design, the sampled covariates are

$$x = \left\{ \begin{array}{c} 18, 19, 20, 34(2), 35(6), 44(3), 45(4), 61(2), 62, 63(3), \\ 64(2), 65, 66(3), 84(3), 85, 103, 106(3), 110, 280. \end{array} \right\}$$

The corresponding design is represented as a histogram in Figure 3 (b). From Figure 1, we can see that the loss decreases for roughly the first 100 generations and then is fairly stable; the algorithm terminated in fewer than 400 generations.

In Fig 2, the designs for different values of δ are represented as histograms. To see the effect of $g_0(x)$ on the design, in Fig 3, we draw the histograms correspondiong to the robust designs in Case 1 for different $g_0(x)$. The components of the loss for the optimal design for different values of δ are shown in Table 1 for $g_0(x) = x$, Table 2 for $g_0(x) = x^2$ and Table 3 for $g_0(x) = x^3$.

To see the effect of the initial distribution $F_0(x)$, we take different $N_h, h = 1, \ldots, L$, in Case 2 and then compare the results with corresponding results in Case 1.

Case 2. $N_1 = 70$, $N_2 = 63$, $N_3 = 98$, $N_4 = 49$, $N_5 = 28$, $N_6 = 30$.

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 $\mathbf{p}^0 = (70/338, 63/338, 98/338, 49/338, 28/338, 30/338)'$. We reran the algorithm, with these strata but the remaining inputs as in Case 1, and found a minimum loss of 27.15 – substantially larger than that in Case 1. The sampled covariates are

$$x = \left\{ \begin{array}{c} 18, 19, 20, 33(2), 34(6), 44(3), 45(8), 66(2), 67(3), \\ 68(2), 69, 82, 84(3), 85, 102(2), 103, 106, 213, \end{array} \right\}$$

which are somewhat different than those in Case 1.

To see the effect of initial $\mathbf{p}^0$, the robust designs in Case 1 and Cases 2 are represented as histograms in Fig 4.

The components of the loss for the optimal design for different values of δ are shown in Table 4 for $g_0(x) = x$, Table 5 for $g_0(x) = x^2$ and Table 6 for $g_0(x) = x^3$. Comparing Table 1 with Table 4, Table 2 with Table 5, and Table 3 with Table 6, we observe that the minimum loss depends heavily on the initial distribution $F_0(x)$.

Now, we compare robust designs with non-robust designs. For the Case 1 of Sugar farm population when $g_0(x) = x$ and $\delta = 0$, applying the algorithm, we obtain the design, denoted by ξ_0, with sampled covariates

$$x = \left\{ \begin{array}{c} 18, 19, 34(3), 35(6), 44(3), 45(3), 61(3), 62, 63(3), \\ 64(2), 65, 66(3), 84(3), 85, 103, 106(3), 263, 280. \end{array} \right\}$$

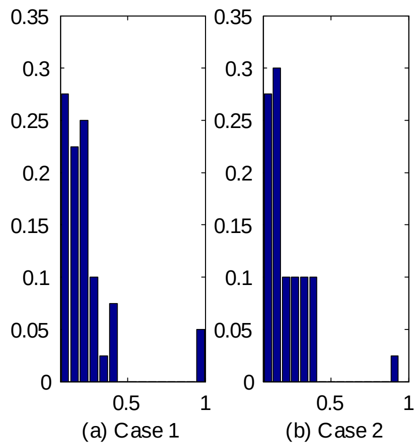

Figure 4: Robust designs for Cases 1 and 2 with $g_0(x) = x^3, \delta = 0.15$

Table 4. Sugar farm: components of loss for Case 2, $g_0(x) = x$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$\mathcal{L}_{0,\delta}$	11.533	15.057	20.208	26.960	35.233	45.053	56.425	69.384	84.221
$\mathcal{L}_v$	0.188	0.189	0.189	0.190	0.190	0.191	0.191	0.192	0.191
$\mathcal{L}_{\max}$	11.721	15.246	20.397	27.150	35.423	45.244	56.62	69.576	84.22

Table 5. Sugar farm: components of loss for Case 2, $g_0(x) = x^2$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$\mathcal{L}_{0,\delta}$	2.478	3.700	5.480	7.798	10.616	13.942	17.770	22.100	26.921
$\mathcal{L}_v$	0.054	0.054	0.054	0.055	0.056	0.056	0.056	0.057	0.056
$\mathcal{L}_{\max}$	2.532	3.754	5.534	7.853	10.672	13.998	17.826	22.157	26.977

Table 6. Sugar farm: components of loss for Case 2, $g_0(x) = x^3$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$\mathcal{L}_{0,\delta}$	0.699	1.134	1.747	2.517	3.451	4.539	5.811	7.248	8.837
$\mathcal{L}_v$	0.018	0.018	0.020	0.021	0.022	0.022	0.023	0.023	0.023
$\mathcal{L}_{\max}$	0.717	1.152	1.767	2.538	3.473	4.571	5.834	7.271	8.860

Table 7. Comparison of robust designs and non-robust designs.

	δ							
	.05	.10	.15	.20	.25	.30	.35	.40
$\mathcal{L}_{\max}$	13.002	16.524	21.039	26.582	33.080	40.593	49.321	59.240
$\mathcal{L}_{\max,\xi_0}$	13.003	16.538	21.20	27.033	34.056	42.278	51.706	62.341

Then we calculate the maximum loss corresponding to ξ_0 for different values of δ, denoted by $\mathcal{L}_{\max,\xi_0}$ in the third row of Table 7. In the second row of Table 7, we list the minimum loss corresponding to robust designs. We can observe that robust designs give us smaller loss than non-robust designs.

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

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

Under the true model (5), $\mathbf{y}_{N-n} = \mathbf{Z}_{N-n}\boldsymbol{\theta} + \mathbf{G}^{1/2}_{N-n}\boldsymbol{\varepsilon}_{N-n}$ and $\hat{\mathbf{y}}_{N-n} = \mathbf{Z}_{N-n}\hat{\boldsymbol{\theta}}$; hence

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

where $\mathbf{M} = \mathbf{Z}_{N-n}(\mathbf{Z}'_n\mathbf{G}^{-1}_{0,n}\mathbf{Z}_n)^{-1}\mathbf{Z}'_n\mathbf{G}^{-1}_{0,n}\mathbf{G}^{1/2}_n$. Then

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

and we find that

$$\begin{aligned}&E_g(\hat{T} - T)^2\\ &= E_g(\mathbf{1}'_{N-n}(\hat{\mathbf{Y}}_{N-n} - \mathbf{Y}_{N-n})(\hat{\mathbf{Y}}_{N-n} - \mathbf{Y}_{N-n})'\mathbf{1}_{N-n})\\ &= \sigma^2\mathbf{1}'_{N-n}[\mathbf{M}\mathbf{M}' + \mathbf{G}_{N-n}]\mathbf{1}_{N-n}\\ &= \sigma^2\mathbf{1}'_{N-n}[(\mathbf{Z}_{N-n}(\mathbf{Z}'_n\mathbf{G}^{-1}_{0,n}\mathbf{Z}_n)^{-1}\mathbf{Z}'_n\mathbf{G}^{-1}_{0,n}\mathbf{G}_n\mathbf{G}^{-1}_{0,n}\mathbf{Z}_n(\mathbf{Z}'_n\mathbf{G}^{-1}_{0,n}\mathbf{Z}_n)^{-1}\mathbf{Z}^{-1}_{N-n} + \mathbf{G}_{N-n}]\mathbf{1}_{N-n}.\end{aligned}$$

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

$$\frac{E_g(\hat{T}-T)^2}{\sigma^2} = \mathbf{1}'_{N-n}\left[\begin{array}{c}(\mathbf{Q}_r\mathbf{Z}_N(\mathbf{Z}'_n\mathbf{G}_{0,n}^{-1}\mathbf{Z}_n)^{-1}\mathbf{Z}'_n\mathbf{G}_{0,n}^{-1}\mathbf{G}_n\cdot \\ \mathbf{G}_{0,n}^{-1}\mathbf{Z}_n(\mathbf{Z}'_n\mathbf{G}_{0,n}^{-1}\mathbf{Z}_n)^{-1}\mathbf{Z}'_N\mathbf{Q}'_r\end{array}\right]\mathbf{1}_{N-n} + \sum_{k\notin s} g\left(x_k\right). \tag{A.1}$$

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

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

hence

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

Since, 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

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

After some simplification we obtain

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

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 from $\mathbf{Z}_N = (\mathbf{Id}_1, \mathbf{Id}_1 * \mathbf{x}_N, \dots, \mathbf{Id}_L, \mathbf{Id}_L * \mathbf{x}_N)$ that

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

with

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

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

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

this in (A.1) give us the desired MSE (7). Finally, we express $C_{h,g}^{k,l}$ in the simpler and more convenient form (8). ■

Proof of Theorem 1: From (7) and (8) we obtain

$$\begin{aligned}
&\frac{E_{g,F}(\hat{T} - T)^2}{\sigma^2} \\
&= \sum_{h=1}^{L}\left(p_h^2 \mathbf{1}_{N-n}'\mathbf{Q}_r\mathbf{C}_{h,g}\mathbf{Q}_r'\mathbf{1}_{N-n} + p_h(1-p_h)\mathbf{1}_{N-n}'\mathbf{Q}_r\mathbf{R}_{h,g}\mathbf{Q}_r'\mathbf{1}_{N-n}\right) + \sum_{k\notin s} g\left(x_k\right) \\
&= \sum_{h=1}^{L}\left(p_h^2\sum_{k\notin s}\sum_{l\notin s} C_{h,g}^{k,l} + p_h(1-p_h)\sum_{k\notin s} C_{h,g}^{k,k}\right) + \sum_{k\notin s} g\left(x_k\right) \\
&= \sum_{h=1}^{L}\sum_{i\in s_h} g(x_i)\left(p_h^2\sum_{k\notin s}\sum_{l\notin s} D_{h,i}^{k,l} + p_h(1-p_h)\sum_{k\notin s} D_{h,i}^{k,k}\right) + \sum_{k\notin s} g\left(x_k\right) \\
&:= S_{g|s} + S_{g|s^c}.
\end{aligned}$$

Since $S_{g|s}$ 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,

$$\max_{g\in\mathcal{G}} \frac{E_{g,F}(\hat{T} - T)^2}{\sigma^2} = \max_{g\in\mathcal{G}} S_{g|s} + \max_{g\in\mathcal{G}} S_{g|s^c}.$$

For the maximum problem out of sample s, we have

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

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

$$\sum_{k\notin s} D_{h,i}^{k,k} \geq 0. \tag{A.3}$$

Similarly,

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

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

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

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,

$$\begin{aligned}&\max_{g\in\mathcal{G}} \frac{E_{g,F}(\hat{T}-T)^2}{\sigma^2}\\ &= (1+\tau_g^2)\left[\sum_{h=1}^{L}\left(p_h^2\left(\sum_{k\notin s}\sum_{l\notin s} C_{h,g_0}^{k,l} - \sum_{k\notin s} C_{h,g_0}^{k,k}\right) + p_h\sum_{k\notin s} C_{h,g_0}^{k,k}\right) + \sum_{k\notin s} g_0\left(x_k\right)\right].\end{aligned}$$

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

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

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

Proof of Theorem 2: Write the constraint (ii) as

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

Denote by $\mathbf{p}_0$ the maximizer, which is guaranteed to exist since 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

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

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 $\mathbf{p}_1$,

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

Condition (A.6) entails

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

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 3: 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 2 satisfies (13), with λ determined by (12) in order to satisfy constraint (i). ■

Proof of Theorem 4: (i) Set $\mathbf{v} = \mathbf{p} - \mathbf{p}^0$. Then

$$\max_{\mathcal{P}^0} \mathbf{p}'\mathbf{B}\mathbf{p} + \mathbf{c}'\mathbf{p} = \mathcal{L}_0 + \mathcal{L}_\delta^0, \tag{A.7}$$

where

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

Thus it suffices to find $\mathcal{L}_\delta^0$. 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

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

with $\mathbf{E} = \mathbf{D}'\mathbf{B}\mathbf{D} : (L-1) \times (L-1)$ and $\mathbf{d} = \mathbf{D}'(\mathbf{B}\mathbf{p}^0 + \mathbf{c}/2) \in \mathbb{R}^{L-1}$. 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 $\mathbf{w}_* = -\mathbf{E}^{-1}\mathbf{d}$ 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 since $-\mathbf{E}$ is positive semidefinite. So, the minimizer is $\mathbf{w} = -\mathbf{E}^{-1}\mathbf{d}$.

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. Since $\mathbf{E}$ is not positive semidefinite or negative semidefinite, the largest eigenvalue λ_1 of 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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