Robust Sampling Designs for Model-Based Stratification

by

Zhichun Zhai

A thesis submitted in partial fulfillment of the requirements for the degree of

Master of Science

in

Statistics

Department of Mathematical and Statistical Sciences
University of Alberta

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 two case studies of Australian sugar farms and MU281 population.

Acknowledgements

I would like to thank my supervisor, Professor Douglas P. Wiens, for his guidance, supervision and encouragement during my master program, which was supported by the Department of Mathematical and Statistical Sciences and Wiens' research grants, at University of Alberta.

Many thanks are due to Professor G. Heo, Professor R.J. Karunamuni, Professor L. Kong, Professor I. Mizera and Professor N. Prasad, who either taught me courses or gave many valuable helps for my studying.

Special thanks go to my family: my mother, parents-in-law, my brother and sister. Their support has provided me the strength to keep myself going. I would like to thank my wife, Rui Hu, not only for her love but also for her confidence in me. Finally, I am thankful to my daughter, Amy Zhai, who keeps me happy and hopeful.

Contents

1 Introduction **1**

1.1 Robustness of design 1

1.2 Robust model-based sampling designs 9

1.3 Model-based stratification 13

1.4 Purpose of this research 16

1.5 Chapter structure 17

2 Neighbourhoods of the working distribution and variance function **18**

3 Maximizing the scaled mean squared error **22**

3.1 The scaled mean squared error with respect to the true distribution and variance function 22

3.2 Maximizing the scaled mean squared error over the neighbourhood of the working variance function 27

3.3 Maximizing the scaled mean squared error over the neighbourhood of the working distribution 30

4 Minimizing the loss function by using a modified genetic algorithm

with artificial implantation **39**

4.1 The genetic algorithm 39

4.2 The modified genetic algorithm with/without artificial implantation . 42

4.3 The sugar farm population 45

4.4 MU281 population 51

4.5 Comparison of the modified genetic algorithm with/without artificial implantation 55

5 Conclusions and future research **59**

Bibliography **61**

List of Figures

4.1 Minimum loss vs. generation Case 1 of sugar farm when $g_0(x) = x, \delta = 0.15$ 46

4.2 Robust designs for Case 1 of sugar farm when $g_0(x) = x^3$ and $\delta = 0, 0.1, 0.2, 0.3$ 47

4.3 Robust designs for Case 1 of sugar farm when $\delta = 0.15$ and $g_0(x) = 1, x, x^2, x^3$ 47

4.4 Robust designs for Cases 1 and 2 of sugar farm when $g_0(x) = x^3, \delta = 0.15$ 49

4.5 Minimum loss vs. generation and best design for Case 1 of MU281 when g(x)=x and $\delta = 0.15$ 53

4.6 Minimum loss vs. generation and best design for Case 2 of MU281 when g(x)=x and $\delta = 0.15$ 54

4.7 Boxplot of minimum losses without/with AI 56

4.8 Boxplot of generations without/with AI 57

4.9 Histogram of generations without AI 58

4.10 Histogram of generations with AI 58

Chapter 1

Introduction

1.1 Robustness of design

In an experiment, the experimenter obtains information on a response variable Y and an independent variable $\mathbf{x}$, which might be a vector, and studies the effect of $\mathbf{x}$ on Y. Usually, the experimenter believes that an assumed model $Y_i = f(\mathbf{x}_i|\boldsymbol{\theta}) + \varepsilon_i$ is true. Here $\boldsymbol{\theta}$ is the vector of unknown parameters and ε_i are random errors. Usually, the experimenter might be able to choose the values of $\mathbf{x}$ from the design space $\boldsymbol{\chi} = \{\mathbf{x}_i\}_{i=1}^N$. In an optimal design problem, the experimenter searches for the levels of $\mathbf{x}$ and wants to allocate observations at those levels of $\mathbf{x}$ so that the unknown parameters in the assumed model are estimated in an optimal manner. But, in most applications, the assumed model is only a reasonable approximation to the true model. Thus, we need the concept of robust design for model misspecifications. Box and Draper (1959) considered the problem of designing for a polynomial response when the true models are such functions of a given higher degree. For example,

suppose that the experimenter is to fit a straight line

$$y_i = \theta_0 + \theta_1 x_i + \varepsilon_i, \quad -1 \leq x \leq 1,$$

but in fact the true model is

$$y_i = \theta_0 + \theta_1 x_i + \theta_2 x_i^2 + \varepsilon_i, \quad -1 \leq x \leq 1.$$

Assume uncorrelated errors with common variance σ_ε^2. Then, the least squares estimate of $\boldsymbol{\theta} = (\theta_0, \theta_1)'$ is

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y},$$

with $\mathbf{X}$ denoting the model matrix with i^{th} row $\mathbf{f}'(x_i) = (1, x_i)$. Define the $k-$th sample moment $\tau_k = \sum_{i=1}^n x_i^k/n$. Let $\tau_1 = \tau_3 = 0$ which is true for symmetric designs. Then, under the true quadratic model, the mean vector and covariance matrix of $\hat{\boldsymbol{\theta}}$ are

$$\begin{aligned} E(\hat{\boldsymbol{\theta}}) &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'E(\mathbf{y}) \\ &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\left(\mathbf{X}\begin{pmatrix}\theta_0\\ \theta_1\end{pmatrix} + \theta_2\begin{pmatrix}x_1^2\\ \vdots\\ x_n^2\end{pmatrix}\right) \\ &= \begin{pmatrix}\theta_0 + \theta_2\tau_2\\ \theta_1\end{pmatrix}, \end{aligned}$$

$$Cov(\hat{\boldsymbol{\theta}}) = \sigma_\varepsilon^2(\mathbf{X}'\mathbf{X})^{-1} = (\sigma_\varepsilon^2)diag(1, \tau_2^{-1}).$$

Then, the predictions $\hat{Y}(x) = (1, x)\hat{\boldsymbol{\theta}}$ have

$$\begin{aligned} E(\hat{Y}(x)) &= (1, x)E(\hat{\boldsymbol{\theta}}) \\ &= (1, x)\begin{pmatrix} \theta_0 + \theta_2\tau_2 \\ \\ \theta_1 \end{pmatrix} \\ &= \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_2\tau_2 - \theta_2 x^2 \\ &= E(Y(x)) + \theta_2(\tau_2 - x^2). \end{aligned}$$

Thus, the predictions $\hat{Y}(x) = (1, x)\hat{\boldsymbol{\theta}}$ have mean squared error

$$MSE(\hat{Y}(x)) = (\sigma_\varepsilon^2)(1 + x^2\tau_2^{-1}) + (\theta_2(\tau_2 - x^2))^2.$$

A common design criterion is the integrated mean squared error (IMSE) of the fitted response. So, here, it is

$$IMSE = \int_{-1}^{1} MSE(\hat{Y}(\mathbf{x}))d\mathbf{x} = \left\{\frac{2\sigma_\varepsilon^2}{n}\left(1 + \frac{1}{3\tau_2}\right)\right\} + \left\{2\theta_2^2\left(\left(\tau_2 - \frac{1}{3}\right)^2 + \frac{4}{45}\right)\right\}.$$

The first term in the **IMSE**, that is the integrated variance, is minimized by the classically optimal design. The second term in the **IMSE**, that is the integrated squared bias dominate the first term when n is sufficiently large. The integrated squared bias is minimized when $\tau_2 = \frac{1}{3}$, which is the second moment of the continuous

uniform distribution on $[-1, 1]$. A design approximating the uniform is the equally spaced design

$$x_i = -1 + 2\frac{i-1}{n-1}, \quad i = 1, 2, \cdots, n$$

with $\tau_2 = \frac{1}{3} + \frac{2}{3(n-1)} = \frac{1}{3} + O(1/n)$.

Generally, the experimenter assumes the model is

$$E(Y(\mathbf{x})) = \mathbf{f}'(\mathbf{x})\boldsymbol{\theta},$$

but the true model is

$$E(Y(\mathbf{x})) = \mathbf{f}'(\mathbf{x})\theta + \psi(\mathbf{x})$$

for some function ψ. To make the parameter θ identifiable, we define the target parameter by

$$\theta = \arg\min_{\boldsymbol{\eta}} \int_{\boldsymbol{\chi}} (E(Y(\mathbf{x})) - \mathbf{f}'(\mathbf{x})\boldsymbol{\eta})^2 d\mathbf{x}.$$

Then define

$$\psi(\mathbf{x}) = E(Y(\mathbf{x})) - \mathbf{f}'(\mathbf{x})\boldsymbol{\theta}$$

which leads to the orthogonality requirement

$$\int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x})\psi(\mathbf{x}) d\mathbf{x} = \mathbf{0}.$$

Thus, under the assumption that $\mathbf{A} = \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x})\mathbf{f}'(\mathbf{x}) d\mathbf{x}$ is invertible, the parameter is

unique

$$\boldsymbol{\theta} = \mathbf{A}^{-1} \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) E(Y(\mathbf{x})) d\mathbf{x}.$$

In the following, we identify a design, denoted by ξ, with its design measure-a probability measure $\xi(d\mathbf{x})$ on $\boldsymbol{\chi}$. Denote

$$\mathbf{M}_\xi = \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) \mathbf{f}'(\mathbf{x}) \xi(d\mathbf{x}),$$

$$\mathbf{b}_{\psi,\xi} = \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) \psi(\mathbf{x}) \xi(d\mathbf{x}).$$

Under the assumption that $\mathbf{M}_\xi$ is invertible, the least squares estimate (lse) $\hat{\boldsymbol{\theta}}$ is

$$\hat{\boldsymbol{\theta}} = \mathbf{M}_{\boldsymbol{\xi}}{}^{-1} \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) Y(\mathbf{x}) \xi(d\mathbf{x}).$$

So, it has expectation

$$\begin{aligned} E(\hat{\boldsymbol{\theta}}) &= \mathbf{M}_{\boldsymbol{\xi}}{}^{-1} \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) E(Y(\mathbf{x})) \xi(d\mathbf{x}) \\ &= \mathbf{M}_{\boldsymbol{\xi}}{}^{-1} \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) (\mathbf{f}'(\mathbf{x})\theta + \psi(\mathbf{x})) \xi(d\mathbf{x}) \\ &= \mathbf{M}_{\boldsymbol{\xi}}{}^{-1} \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) \mathbf{f}'(\mathbf{x}) \boldsymbol{\theta} \xi(d\mathbf{x}) + \mathbf{M}_{\boldsymbol{\xi}}{}^{-1} \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) \psi(\mathbf{x}) \xi(d\mathbf{x}) \\ &= \boldsymbol{\theta} + \mathbf{M}_\xi^{-1} \mathbf{b}_{\psi,\xi} \end{aligned}$$

and bias $\mathbf{M}_\xi^{-1} \mathbf{b}_{\psi,\xi}$. The covariance matrix of the lse $\hat{\boldsymbol{\theta}}$ is $(\sigma_\varepsilon^2/n) M_\xi^{-1}$. Thus the **IMSE**

of the prediction $\hat{Y}(\mathbf{x})$ is

$$IMSE = \int_{\boldsymbol{\chi}} MSE(\hat{Y}(\mathbf{x}))d\mathbf{x} = \frac{\sigma_\varepsilon^2}{n}\mathbf{trace}(A\mathbf{M}_\xi^{-1}) + \mathbf{b}'_{\psi,\xi}\mathbf{M}_\xi^{-1}A\mathbf{M}_\xi^{-1}\mathbf{b}_{\psi,\xi} + \int_{\boldsymbol{\chi}} \psi^2(\mathbf{x})d\mathbf{x}. \tag{1.1}$$

Huber (1975) studied approximate straight line regression. But the true model was

$$E(Y(\mathbf{x})) = \mathbf{f}'(x)\boldsymbol{\theta} + \psi(x)$$

with $\mathbf{f}(x) = (1, x)', x \in \boldsymbol{\chi} = [-1/2, 1/2]$, ψ in the class

$$\Psi = \left\{\psi : \int_{\boldsymbol{\chi}} \psi^2(x)dx \leq \tau^2/n, \int_{\boldsymbol{\chi}} \mathbf{f}(x)\psi(x)dx = 0\right\} \tag{1.2}$$

for a given constant τ. Huber used the **IMSE** as the design criterion and found optimal 'minimax' designs (maximize over ψ, then minimize over ξ). The class Ψ was criticized (Marcus and Sacks (1976), Li and Notz (1982)) as being too wide. It was claimed in these papers, and proved in Wiens (1992), that any implementable and non-randomized, hence discrete, design has infinite maximum loss in the Ψ.

Marcus and Sacks (1976), Sacks and Ylvisaker (1978), Pesotchinsky (1982), Li and Notz (1982) and Li (1984) considered ψ from the class

$$\Psi = \{\psi : |\psi(x)| \leq \phi(x), x \in \chi\}$$

with various assumptions being made about ϕ. The optimal designs constructed in these papers appear to be quite sensitive to the assumed form of ϕ. Their class Ψ

seems to be rather thin. The designs mass tends to concentrate at some extreme points of the design space. So the resulting designs are not 'robust' because there is no way to explore the interior of the design space.

Usually, to obtain a robust design with respect to the class Ψ in (1.2), we maximize the **IMSE** in (1.1) over the class Ψ and then minimize the maximum in the first step over the class of designs. Generally, as explained by Wiens (2014), the maximum over the class Ψ of **IMSE** has the form

$$\max_{\Psi} \text{IMSE} = \frac{\sigma_\varepsilon^2 + \tau^2}{n} \mathcal{L}_\nu(\xi)$$

with $\nu = \tau^2/(\sigma_\varepsilon^2 + \tau^2)$ and

$$\mathcal{L}_\nu(\xi) = [(1-\nu)\text{trace}(\mathbf{A}\mathbf{M}_\xi^{-1}) + \nu \text{ch}_{\max}(\mathbf{K}_\xi \mathbf{H}_\xi^{-1})].$$

Here $\text{ch}_{\max}$ denotes the maximum eigenvalue,

$$\mathbf{H}_\xi = \mathbf{M}_\xi \mathbf{A}^{-1} \mathbf{M}_\xi$$

and

$$\mathbf{K}_\xi = \int_{\boldsymbol{\chi}} \mathbf{f}(\mathbf{x}) \mathbf{f}'(\mathbf{x}) m^2(\mathbf{x}) d\mathbf{x}$$

with $m(x)$ the density of ξ. Then, the next step is minimizing $\mathcal{L}_\nu(\xi)$ for a given ν which is the weight for errors due to bias. In some cases, this step can be done analytically, see Huber (1981) and Wiens (1990). But in other cases, such as examples

given by Wiens (1990,1992), it is difficult to determine which one of the eigenvalues $e_1(\xi), \ldots, e_p(\xi)$ of $\mathbf{K}_\xi \mathbf{H}_\xi^{-1}$ is the maximum one. Usually, one chooses an eigenvalue to be optimized and then to verify it is the maximum eigenvalue. But, there are cases in which this approach does not work. Daemi and Wiens (2013) introduced an alternative method for construction of robust regression design. Shi, Ye and Zhou (2003) applied Lagrange multiplier rule from nonsmooth optimization to minimize the non-differentiable functional $\mathcal{L}_\nu(\xi)$. Heo et al. (2001) considered smaller class of designs with densities of the form $m_{\boldsymbol{\beta}} = \max(0, \sum_j \beta_j f_j(x_1^2, \cdots, x_q^2))$, where in the true model $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \cdots, f_p(\mathbf{x}))'$. Then, they minimized $\mathcal{L}_\nu(\xi)$ numerically over $\boldsymbol{\beta}$ subject to the condition that the arguments of m be exchangeable.

1.2 Robust model-based sampling designs

Consider a finite population of N units in which a survey variable Y has population values $Y_1, \cdots, Y_N$ and a $q-$dimensional auxiliary variable $\mathbf{x}$ has known population values $\mathbf{x}_1, \cdots, \mathbf{x}_N$. In a sample s with sample size $n \leq N$, we assume that all n units of Y in s are known. The estimation/prediction problem is to use $Y_i, i \in s$ and $\mathbf{x}_1, \cdots, \mathbf{x}_N$ to estimate or predict the unknown finite population total $T = \sum_{i=1}^N Y_i$ based on a linear relationship-possibly transformed- between Y and given functions of $\mathbf{x}$. The design problem is to determine which values of $\mathbf{x}$ will be selected in the sample so that the estimation or prediction has optimal properties. When studying the model-based design, the estimation/prediction problem and the design problem can not be considered separately because the choice of estimator or predictor and

the choice of design depend on each other. Thus, the model-based design depends strongly on the assumed relationship. Welsh and Wiens (2013) developed robust model-based designs for a general class of models.

Welsh and Wiens (2013) assumed the working model is

$$\gamma^{-1}(Y_i) = \mathbf{z}'(\mathbf{x}_i)\boldsymbol{\theta} + \sigma_\varepsilon g_0(\mathbf{x}_i)^{1/2}\varepsilon_i. \tag{1.3}$$

Here γ is a known, nonlinear, monotonic transformation, $\mathbf{z}(\mathbf{x}_i)$ is a $p-$dimensional vector of regressors, $\boldsymbol{\theta}$ is an unknown $p-$dimensional regression parameter, σ_ε is an unknown non-negative scale parameter, $g_0 : \mathbb{R}^q \longrightarrow \mathbb{R}^+$ is a known, positive variance function and $\{\varepsilon_1, \cdots, \varepsilon_N\}$ are independent and identically distributed random variables with mean zero and variance one. Welsh and Wiens (2013) assumed that model (1.3) is only an approximation to the following model

$$\gamma^{-1}(Y_i) = \mathbf{z}'(\mathbf{x}_i)\boldsymbol{\theta} + f(\mathbf{x}_i) + \sigma_\varepsilon g(\mathbf{x}_i)^{1/2}\varepsilon_i + \eta(\mathbf{x}_i). \tag{1.4}$$

Here $f : \mathbb{R}^q \longrightarrow \mathbb{R}$ is a function representing departures from the linear mean function, $g : \mathbb{R}^q \longrightarrow \mathbb{R}^+$ is known, positive function representing departures from the variance function when $g \neq g_0$, and $\eta(\mathbf{x})$ is a random process with mean zero and covariance function $\text{COV}\{\eta(\mathbf{x}, \eta(\mathbf{x}')\} = h(\mathbf{x}, \mathbf{x}')$ representing departures from inde-

pendence. Denote

$$\mathbf{Z}_N = \begin{pmatrix} \mathbf{z}'(\mathbf{x}_1) \\ \vdots \\ \mathbf{z}'(\mathbf{x}_N) \end{pmatrix}, \quad \mathbf{f}_N = \begin{pmatrix} \mathbf{f}(\mathbf{x}_1) \\ \vdots \\ \mathbf{f}(\mathbf{x}_N) \end{pmatrix},$$

$$\boldsymbol{\varepsilon}_N = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_N \end{pmatrix}, \quad \boldsymbol{\eta}_N = \begin{pmatrix} \boldsymbol{\eta}(\mathbf{x}_1) \\ \vdots \\ \boldsymbol{\eta}(\mathbf{x}_N) \end{pmatrix}.$$

Denote $\mathbf{G}_{0,N} = \text{diag}\{g_0(\mathbf{x}_1), \cdots, g_0(\mathbf{x}_N)\}$ and $\mathbf{G}_N = \text{diag}\{g(\mathbf{x}_1), \cdots, g(\mathbf{x}_N)\}$. Let $\mathbf{H}_N$ be the $N \times N$ matrix with $(k,l)^{th}$ element $h(\mathbf{x}_k, \mathbf{x}_l)$. Denote $\boldsymbol{\delta} = (\gamma^{-1}(Y_1), \cdots, \gamma^{-1}(Y_N))'$. Then $\boldsymbol{\delta}$ has the first two moments

$$E(\boldsymbol{\delta}) = \mathbf{Z}_N\boldsymbol{\theta} + \mathbf{f}_N \quad \text{and} \quad \text{Cov}(\boldsymbol{\delta}) = \sigma_\varepsilon^2\mathbf{G}_N + \mathbf{H}_N.$$

To make the parameter θ identifiable, we define the target parameter by

$$\boldsymbol{\theta} = \arg\min_{\boldsymbol{\phi}} \sum_{i=1}^{N} [E_{\varepsilon,\eta}\{\gamma^{-1}(Y_i - \mathbf{z}'(\mathbf{x}_i))\boldsymbol{\phi}\}]^2.$$

Assume $\sum_{i=1}^{N} \mathbf{z}(\mathbf{x}_i))\mathbf{z}'(\mathbf{x}_i))$ is invertible. Then, the definition of $\boldsymbol{\theta}$ leads to the orthogonality condition

$$\mathbf{Z}_N'\mathbf{f}_N = \sum_{i=1}^{N} \mathbf{z}(\mathbf{x}_i) f(\mathbf{x}_i) = \mathbf{0}.$$

Welsh and Wiens (2013) studied model (1.4) in the following neighbourhoods of

f, g, h, respectively,

$$\mathcal{F} = \{f : \mathbb{R}^q \longrightarrow \mathbb{R} : \mathbf{Z}_N'\mathbf{f}_N = \mathbf{0} \quad \text{and} \quad \mathbf{f}_N'\mathbf{f}_N \leq \tau_f^2\},$$

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

$$\mathcal{H} = \{\mathbf{H} : \mathbf{H} \text{ positive semi-definite and} \|\mathbf{H}\| \leq \tau_H^2/N\}.$$

Here $\|\cdot\|$ is any induced matrix norm. For the scaled prediction mean squared error

$$\frac{E(T - \hat{(T)})^2}{N\{\tau_f^2 + \sigma_\varepsilon^2(1 + \tau_g^2) + \tau_h^2\}},$$

Welsh and Wiens (2013) derived an upper bound

$$\mathcal{L}_N(f, g, h) = \frac{(nN)^{-1} \sum_{i \notin s} g_0(\mathbf{x}_i) \sum_{j \in s} E[g_0^{-1/2}(\mathbf{x}_i)r_i - g_0^{-1/2}(\mathbf{x}_j)r_j]^2}{\tau_f^2 + \sigma_\varepsilon^2(1 + \tau_g^2) + \tau_h^2}.$$

Here $r_i = \gamma^{-1}(Y_i) - \mathbf{z}'(\mathbf{x}_i)\hat{\boldsymbol{\theta}}$ with the weighted least squares estimator $\hat{\boldsymbol{\theta}}$ of the regression parameter $\boldsymbol{\theta}$ in model (1.3):

$$\hat{\boldsymbol{\theta}} = \left[\sum_{j \in s} \mathbf{z}(\mathbf{x}_j)\mathbf{z}'(\mathbf{x}_j)/g_0(\mathbf{x}_j)\right]^{-1} \sum_{j \in s} \mathbf{z}(\mathbf{x}_j)\gamma^{-1}(Y_j)/g_0(\mathbf{x}_j).$$

Then, they adopted a minimax approach to choose the design to minimize the maximum of $\mathcal{L}_N(f, g, h)$ over the neighbourhoods $\mathcal{F}, \mathcal{G}, \mathcal{H}$.

1.3 Model-based stratification

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.*

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:

$$E(y_i | i \in h) = \mu_h, \ \text{VAR}(y_i | i \in h) = \sigma_h^2,$$

$$y_i \text{ and } y_j \text{ are independent when } i \neq j.$$

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 $\sum_h (N_h^2/n_h)(1 - n_h/N_h)\hat{\sigma}^2_{n_h}$ where $\hat{\sigma}^2_{n_h} = \frac{1}{n_h}\sum_{i \in s_h}(y_i - \overline{y}_{n_h})^2$ 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 lies in the h^{th} strata provided the corresponding $x_i \in (F_0^{-1}(a_{h-1}), F_0^{-1}(a_h))$. (1.5)

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:

$$Y_i = \alpha_h + \beta_h x_i + g_0^{1/2}(x_i)\varepsilon_i, \ i \in h, \ h = 1, \cdots, L. \tag{1.6}$$

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. Model (1.6) is more general than model (5.14) studied in Chambers and Clark (2012). Special cases of model (1.6) have been studied by many researchers. Bethel (1989) used model (1.6) with parameters independent on strata to study some estimators in model-based stratification. Based on a similar model, Kott (1985) improved the results in Godfrey et at. (1984).

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) $E(T - \hat{T})^2$.

1.4 Purpose of this research

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. Specifically, for any distribution function $F(\cdot)$ and variance function $g(\cdot)$ near the working distribution $F_0(\cdot)$ and variance function $g_0(\cdot)$, we fist find the MSE of the estimator/predictor $\hat{T}$ with respect to $F(\cdot)$ and $g(\cdot)$. Roughly speaking, for fixed $F(\cdot)$, the MSE will linearly depend on the values of $g(\cdot)$ at in-sample units and the values of $g(\cdot)$ at non-sample units. For fixed $g(\cdot)$, the MSE

is a quadratic form of the probabilities of strata under the distribution function $F(\cdot)$. Then, the maximum of the MSE over the neighbourhood consisting of $g(\cdot)$ controlled by $g_0(\cdot)$ will be attained at the boundary of the neighbourhood. The maximum problem of the MSE over the neighbourhood of the working distribution $F_0(\cdot)$ turns out to be a constrained quadratic optimization problem. To solve this problem, we will present a method which is convenient for numerical work. We will use a modified genetic algorithm to find the robust design which minimize the maximum of the MSE over the neighbourhoods of the working distribution and variance function.

1.5 Chapter structure

The rest of this thesis is organized as follows. In Chapter 2, we will define neighbourhoods of the working distribution and variance function. In Chapter 3, we will maximize the scaled mean squared error over the neighbourhoods of working variance function and distribution. In Chapter 4, for sugar farm population and MU281 population, applying a modified genetic algorithm, we will find robust designs in different cases.

Chapter 2

Neighbourhoods of the working distribution and variance function

Assume that the population is divided into L strata by applying (1.5). Denote by $\mathbf{Id}_h = (Id_{h1}, \ldots, Id_{hN})'$ the indicator vector of the h^{th} strata. Here $Id_{hi} = 1$ 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 $\boldsymbol{\theta} = (\alpha_1, \beta_1 \ldots \alpha_L, \beta_L)^T$. Then, we can rewrite the working model (1.6) as

$$\mathbf{y}_N = \mathbf{Z}_N \boldsymbol{\theta} + \mathbf{G}_{0,N}^{1/2} \boldsymbol{\varepsilon}_N. \tag{2.1}$$

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

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 $\mathbf{p}^0 = \mathbf{p}_{F_0}$,

$$\mathcal{P} = \{\mathbf{p} \mid \left\|\mathbf{p} - \mathbf{p}^0\right\| \leq \delta; \mathbf{p} \gtrsim \mathbf{0}, \mathbf{1}_L'\mathbf{p} = 1\}, \tag{2.2}$$

and then defining $\mathcal{F}$ to consist of those distributions with $\mathbf{p}_F \in \mathcal{P}$. (We use $\mathbf{p} \gtrsim \mathbf{0}$ 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 (2.1), the true model is now

$$\mathbf{y}_N = \mathbf{Z}_N\boldsymbol{\theta} + \mathbf{G}_N^{1/2}\boldsymbol{\varepsilon}_N, \tag{2.3}$$

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

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 (2.1), 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 (2.1), 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 (2.3) 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 chapter we concentrate on obtaining this maximum scaled mean squared

error

$$\mathcal{L}_{\max} = \max_{F \in \mathcal{F}} \max_{g \in \mathcal{G}} \frac{E_{g,F}(\hat{T} - T)^2}{N\sigma^2(1 + \tau_g^2)}. \tag{2.4}$$

Chapter 3

Maximizing the scaled mean squared error

We will study the optimization problem of obtaining $\mathcal{L}_{\max}$, given by (2.4). 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 $E_{g,F}(\hat{T} - T)^2$.

3.1 The scaled mean squared error with respect to the true distribution and variance function

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

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

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*

$$\frac{E_{g,F}(\hat{T}-T)^2}{\sigma^2} = \mathbf{1}'_{N-n}\mathbf{Q}_r \sum_{h=1}^{L} \left(p_h^2\mathbf{C}_{h,g} + p_h(1-p_h)\mathbf{R}_{h,g}\right)\mathbf{Q}'_r\mathbf{1}_{N-n} + \mathbf{1}'_{N-n}\mathbf{G}_{N-n}\mathbf{1}_{N-n}. \tag{3.1}$$

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*

$$C_{h,g}^{k,l} = \sum_{i\in s_h} g(x_i)D_{h,i}^{k,l}, \tag{3.2}$$

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

Proof. 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 (2.3), $\mathbf{y}_{N-n} = \mathbf{Z}_{N-n}\boldsymbol{\theta} + \mathbf{G}_{N-n}^{1/2}\boldsymbol{\varepsilon}_{N-n}$ and $\hat{\mathbf{y}}_{N-n} = \mathbf{Z}_{N-n}\hat{\boldsymbol{\theta}}$, hence

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

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

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

and we find that

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

With $\mathbf{Q}_r$ as defined in the statement of the Lemma,

$$\frac{E_g(\hat{T} - T)^2}{\sigma^2} = \mathbf{1}_{N-n}'\begin{bmatrix} (\mathbf{Q}_r\mathbf{Z}_N(\mathbf{Z}_n'\mathbf{G}_{0,n}^{-1}\mathbf{Z}_n)^{-1}\mathbf{Z}_n'\mathbf{G}_{0,n}^{-1}\mathbf{G}_n\cdot \\ \mathbf{G}_{0,n}^{-1}\mathbf{Z}_n(\mathbf{Z}_n'\mathbf{G}_{0,n}^{-1}\mathbf{Z}_n)^{-1}\mathbf{Z}_N'\mathbf{Q}_r' \end{bmatrix}\mathbf{1}_{N-n} + \mathbf{1}_{N-n}'\mathbf{G}_{N-n}\mathbf{1}_{N-n}. \tag{3.3}$$

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

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

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

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

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

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

with

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

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 (3.3) give us the desired MSE (3.1). Finally, we express $C_{h,g}^{k,l}$ in the simpler and more convenient form (3.2). ■

3.2 Maximizing the scaled mean squared error over the neighbourhood of the working variance function

We now maximize (3.1) over $g \in \mathcal{G}$.

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

$$\max_{g\in\mathcal{G}} \frac{E_{g,F}(\hat{T}-T)^2}{N\sigma^2(1+\tau_g^2)} = \frac{\mathbf{p}_F'\mathbf{B}\mathbf{p}_F + \mathbf{c}'\mathbf{p}_F + \mathbf{1}_{N-n}'\mathbf{G}_{0,N-n}\mathbf{1}_{N-n}}{N}. \tag{3.4}$$

Here $\mathbf{B} = \text{diag}\{b_h : h = 1, \ldots, L\}$ *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

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

Proof. From (3.1) and (3.2) we obtain

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

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

$$\max_{g\in\mathcal{G}} S_{g|s^c} = \max_{g\in\mathcal{G}}\sum_{h=1}^{L}\sum_{i\notin s_h} g(x_i) = (1+\tau_g^2)\sum_{i\notin s} g_0(x_i), \tag{3.5}$$

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

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

$$\sum_{k\notin s} D_{h,i}^{k,k} \geq 0. \tag{3.6}$$

Similarly,

$$\sum_{k\notin s}\sum_{l\notin s} D_{h,i}^{k,l} = U_{3hi}\left(\sum_{k\notin s} x_k\right)^2 + 2(N-n)U_{2hi}\left(\sum_{k\notin s} x_k\right) + (N-n)^2 U_{1hi} \geq 0. \tag{3.7}$$

Note also that $p_h(1-p_h) \geq 0$ for all h. Then using (3.6) and (3.7), we have

$$\begin{aligned}\max_{g\in\mathcal{G}} S_{g|s} &= \max_{g\in\mathcal{G}}\left(\sum_{h=1}^{L}\sum_{i\in s_h} g(x_i)\left(p_h^2\sum_{k\notin s}\sum_{l\notin s} D_{h,i}^{k,j} + p_h(1-p_h)\sum_{k\notin s} D_{h,i}^{k,k}\right)\right). \\ &= (1+\tau_g^2)\sum_{h=1}^{L}\sum_{i\in s_h} g_0(x_i)\left(p_h^2\sum_{k\notin s}\sum_{l\notin s} D_{h,i}^{k,j} + p_h(1-p_h)\sum_{k\notin s} D_{h,i}^{k,k}\right) \end{aligned} \tag{3.8}$$

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

Combining (3.5) and (3.8) we obtain, after a rearrangement,

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

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

$$\max_{g\in\mathcal{G}} \frac{E_{g,F}(\hat{T}-T)^2}{\sigma^2(1+\tau_g^2)} = \mathbf{p}_F'\mathbf{B}\mathbf{p}_F + \mathbf{c}'\mathbf{p}_F + \mathbf{1}_{N-n}'\mathbf{G}_{0,N-n}\mathbf{1}_{N-n},$$

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

3.3 Maximizing the scaled mean squared error over the neighbourhood of the working distribution

Following Theorem 2 we continue the development by maximizing (3.4) over the neighbourhood $\mathcal{F}$ of $F_0(\cdot)$. For this it suffices to find the maximum value

$$\mathcal{L}_{0,\delta} = \max_{\mathcal{P}} \frac{\mathbf{p}'\mathbf{B}\mathbf{p} + \mathbf{c}'\mathbf{p}}{N}, \tag{3.9}$$

since then

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

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

For simple population, when $L = 2$, we can find the maximum of (3.9) and $\mathcal{L}_{\max}$ easily.

Example 3 *Consider* $x = \{0.1, 0.2, 0.3, 0.6, 0.8, 0.9\}$ *with* $N = 6$. *Take* $N_1 = N_2 = 3$, $L = 2$, $n_1 = n_2 = 2$ *and* $n = 4$. *We assume that* $g_0(x) = x$, $\mathbf{P}^0 = (0.5, 0.5)'$ *and* $\delta = \sqrt{0.5}$. *We can find* $\mathcal{L}_{\max}$ *as follows. When sample* $s = \{0.1, 0.3, 0.6, 0.9\}$, $\mathbf{B} = \text{diag}\{0.8, -0.6667\}$ *and* $\mathbf{c} = (4.4, 5.3333)'$. *So,*

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

and $\mathcal{L}_v = \frac{1}{6}$. *Thus,* $\mathcal{L}_{\max} = 1.0333$.

We list $\mathcal{L}_{\max}$ *for different chooses of samples in table 3.1.*

Table 3.1 Calculation of $\mathcal{L}_{\max}$ for 9 possible samples in Example 3

Sample	(b_1, b_2)	(c_1, c_2)	$\mathcal{L}_{\max}$
$\{0.1, 0.2, 0.6, 0.8\}$	$(7.8, -5.1)$	$(18.6, 7.5)$	4.6
$\{0.1, 0.2, 0.6, 0.9\}$	$(6.8, -0.4,)$	$(14.3, 3.7667)$	3.7
$\{0.1, 0.2, 0.8, 0.9\}$	$(4.8, 46.8)$	$(7.5, 62.1)$	16.7
$\{0.1, 0.3, 0.6, 0.8\}$	$(0.9, -6.6)$	$(5.8, 10.55)$	1.3636
$\{0.1, 0.3, 0.6, 0.9\}$	$(0.8, -0.6667)$	$(4.4, 5.3333)$	1.0333
$\{0.1, 0.3, 0.8, 0.9\}$	$(0.6, 51.2)$	$(2.2, -82.4)$	22.4
$\{0.2, 0.3, 0.6, 0.8\}$	$(-9, -8.1)$	$(23, 14.3)$	2.7107
$\{0.2, 0.3, 0.6, 0.9\}$	$(-7.6, -1.6)$	$(16.9, 15.55)$	2.5688
$\{0.2, 0.3, 0.8, 0.9\}$	$(-4.8, 63.6)$	$(7.7, 106.1)$	28.4

In the following, we want to solve (3.9) analytically.

Theorem 4 *There exists a solution* $\mathbf{p}_0$ *to the problem*

$$\textit{maximize } \mathbf{p}'\mathbf{B}\mathbf{p}+\mathbf{c}'\mathbf{p}\textit{, subject to (i) } \mathbf{1}'\mathbf{p}=1\textit{, (ii) } \left\|\mathbf{p}-\mathbf{p}^0\right\| \leq \delta\textit{, (iii) } \mathbf{p} \succsim \mathbf{0}. \quad (3.10)$$

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).

Proof. Write the constraint (ii) as

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

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

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

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 $\mathbf{p}_1$,

$$0 \geq \Phi'(0;\mu,\lambda) = \left(-2(\mu\mathbf{I} - \mathbf{B})\,\mathbf{p}_0 + \mathbf{c} - 2\lambda\mathbf{1} + 2\mu\mathbf{p}^0\right)'(\mathbf{p}_1 - \mathbf{p}_0). \tag{3.11}$$

Condition (3.11) entails

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

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

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). ■

If δ is sufficiently small, then Theorem 4 can be made much more explicit.

Theorem 5 *If $\delta \leq \min_h p_h^0$, the maximum value $\mathcal{L}_{0,\delta}$ at (3.9) can be obtained as follows. Define*

$$\lambda = \lambda(\mu) = \sum_h (b_h p_h^0 + c_h/2)\alpha_h(\mu), \tag{3.12}$$

for coefficients $\alpha_h(\mu) = (\mu - b_h)^{-1} / \sum_h (\mu - b_h)^{-1}$. Then the maximizing $\mathbf{p}_0$ of Lemma 4 has elements

$$p_{0,h}(\lambda, \mu) = \frac{\mu p_h^0 + c_h/2 - \lambda(\mu)}{\mu - b_h}, \tag{3.13}$$

and

$$\mathcal{L}_{0,\delta} = \max_\mu \frac{\sum_h p_{0,h}(\lambda(\mu), \mu)(b_h p_{0,h}(\lambda(\mu), \mu) + c_h)}{N}, \tag{3.14}$$

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

Proof. If $\delta \leq \min_h p_h^0$ then $\mathbf{p} \gtrsim \mathbf{0}$ for all $\mathbf{p}$ for which $\|\mathbf{p} - \mathbf{p}^0\| \leq \delta$; in particular the solution given by Theorem 4 satisfies (3.13), with λ determined by (3.12) in order to satisfy constraint (i). ■

Even when $\delta \leq \min_h p_h^0$, Theorems 4 and 5 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 (3.10) 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

$$\max_{\|\mathbf{w}\|=\delta} \left(\mathbf{w}'\mathbf{E}\mathbf{w} + 2\mathbf{d}'\mathbf{w}\right), \tag{3.15}$$

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

Lemma 6 *(Hager 2001) The vector* $\mathbf{w}$ *is a solution vector for (3.15) 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 (3.15) 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 $c_i = \frac{\nu_i}{\mu-\lambda_i}$, $1 \le i \le L-1$, *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 (3.9).

Theorem 7 *Denote by* $\mathcal{P}^0$ *the class* $\mathcal{P}$ *defined at (2.2), without the non-negativity requirement* $\mathbf{p} \gtrsim \mathbf{0}$. *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 6, 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 $\mathbf{p}_0 \gtrsim \mathbf{0}$ *then* $\mathbf{p}_0$ *is also the maximizer in* $\mathcal{P}$, *and*

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

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

$$\max_{\mathcal{P}^0} \mathbf{p}'\mathbf{B}\mathbf{p} + \mathbf{c}'\mathbf{p} = \mathcal{L}_0 + \mathcal{L}_\delta^0, \tag{3.16}$$

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

$$\mathcal{L}_\delta^0 = \max_{\|\mathbf{w}\|\leq\delta} \mathbf{w}'\mathbf{E}\mathbf{w} + 2\mathbf{d}'\mathbf{w}, \tag{3.17}$$

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 (3.17) then

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

is a solution to Problem (3.16).

Problem (3.17) 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 (3.17) is either $\mathbf{w}_* = -\mathbf{E}^{-1}\mathbf{d}$ or the solution to (3.15). For this, we consider the following three possibilities:

Case 1: $\mathbf{E}$ is positive semidefinite. In this case (3.17) is a problem of maximizing a convex function over a convex set. According to Corollary 32.3.2 of Rockafellar (1970), the solution of (3.17) must be a boundary point of $\|\mathbf{w}\| \leq \delta$. Thus it suffices to solve (3.15).

Case 2: $\mathbf{E}$ is negative semidefinite. If the maximizer $\mathbf{w}$ of (3.17) 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 (3.17) 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 imme-

diate. ■

Chapter 4

Minimizing the loss function by using a modified genetic algorithm with artificial implantation

4.1 The genetic algorithm

We will use a modified genetic algorithm with artificial implantation to find the optimal robust design which minimizes the loss. For more details for the genetic algorithm, see Mandal et al. (2007) and Welsh and Wiens (2013). We first recall the genetic algorithm as follows.

1. Start by randomly generating the first generation of $n_g = 40$ designs.

2. For the current generation of designs, compute the loss $\mathcal{L} = \mathcal{L}_{N,\delta,k}$ for each

design, $k = 1, \ldots, n_g$, and the corresponding 'fitness levels'

$$\text{fitness}_k = \frac{1}{(\mathcal{L}_{N,\delta,k} - .999\mathcal{L}_{N,\delta,min})^2}, \qquad k = 1, \ldots, n_g,$$

where $\mathcal{L}_{N,\delta,min}$ is the minimum value of the loss in the current generation. Then, scale the fitness levels $\{\text{fitness}_k\}_{k=1}^{n_g}$ to form a probability distribution

$$\psi_k = \frac{\text{fitness}_k}{\sum_{j=1}^{g} \text{fitness}_j}, \qquad k = 1, \ldots, n_g.$$

3. Form a new generation of n_g designs to replace the current generation in the following way.

   (a) Include the fittest $N_{elite} = n_g \times P_{elite}$ of the current generation; they are the elite group which survives through to the next generation. The remaining $n_g - N_{elite}$ members are formed by 'crossover' and 'mutation'. (We used $P_{elite} = .05$, so that $N_{elite} = 2$ and $n_g - N_{elite} = 38$.)

   (b) Crossover proceeds as follows:

   - Choose two members of the current generation to be parents with probability proportional to their fitness level: If $\zeta_1, \zeta_2 \sim$ independent Uniform(0,1), then choose to be parents the current generation members i_1^* and i_2^*, where

$$i_1^* = \min\left\{ i : \sum_{j=1}^{i} \psi_j \geq \zeta_1 \right\} \qquad \text{and} \qquad i_2^* = \min\left\{ i : \sum_{j=1}^{i} \psi_j \geq \zeta_2 \right\}.$$

- With probability $1 - P_{crossover}$, the child is identical to the fittest parent. (We used $1 - P_{crossover} = 0.1$.)
- With probability $P_{crossover}$, the parents both contribute towards the child, in the following manner. Each member of the current generation can be represented by a vector of $N - n$ zeros and n ones, with a one indicating that the corresponding unit is included in the sample. The two vectors arising from the parents are summed, resulting in a vector with elements in $\{0, 1, 2\}$. The sum vector is adjusted to have exactly n non-zero elements by randomly (uniformly) choosing an appropriate number of the ones and replacing them by zeros. Any twos are changed to ones (which means that any points common to both parents are retained). The child formed in this way is added to the new generation.
- Mutation is applied independently n times to each child - regardless of how the child is formed - as follows. For each mutation, randomly choose a one and a zero. Then, with probability $P_{mutation}$, swap the zero and the one and with probability $1 - P_{mutation}$ do nothing. (We used $P_{mutation} = 0.05$.)

The procedure is repeated until n_g members of the new generation are formed.

4. Step 3 is carried out until the next generation has been formed. Then its fitness levels are computed and the process is repeated from Step 2. The loss is

guaranteed to decrease (weakly) in each generation, because of the inclusion of the elite members. We run the algorithm until the best design has not changed in 200 consecutive generations.

4.2 The modified genetic algorithm with/without artificial implantation

Recall that a stratified random sample is obtained as follows: we take independently one 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 $n = \sum_h n_h$. To apply the genetic algorithm to stratified random samples, we need to modify the crossover and mutation procedures in the genetic algorithm to guarantee that in the sample size in h^{th} stratum is n_h. Moreover, we could add a step called artificial implantation (**AI**) to the genetic algorithm. To do **AI** in each generation, 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 the largest stratum in the best design. We present the modified genetic algorithm as follows.

1. Start by randomly generating the first generation of $n_g = 40$ designs.

2. For the current generation of designs, compute the loss $\mathcal{L} = \mathcal{L}_{N,\delta,k}$ for each design, $k = 1, \ldots, n_g$, and the corresponding original 'fitness levels'

$$\text{fitness}_k = \frac{1}{(\mathcal{L}_{N,\delta,k} - .999\mathcal{L}_{N,\delta,min})^2}, \qquad k = 1, \ldots, n_g,$$

where $\mathcal{L}_{N,\delta,min}$ is the minimum value of the loss in the current generation. Then, scale the fitness levels $\{\text{fitness}_k\}_{k=1}^{n_g}$ to form a probability distribution

$$\psi_k = \frac{\text{fitness}_k}{\sum_{j=1}^{g} \text{fitness}_j}, \qquad k = 1, \ldots, n_g.$$

3. Form a new generation of n_g designs to replace the current generation in the following way.

   (a) Include the fittest $N_{elite} = n_g \times P_{elite}$ of the current generation; they are the elite group which survives through to the next generation. The remaining $n_g - N_{elite}$ members are formed by 'crossover' and 'mutation'. (We used $P_{elite} = .05$, so that $N_{elite} = 2$ and $n_g - N_{elite} = 38$.)

   (b) **Artificial Implantation (AI)** Find the largest stratum Str of the fittest design in the current generation. Replace the corresponding strata in all $n_g - 1$ designs by Str in the current generation. The resulted designs together with the fittest design form the current generation with artificial implantation.

   (c) Crossover proceeds as follows:

   - Choose two members of the current generation with artificial implantation to be parents with probability proportional to their original fitness level: If $\zeta_1, \zeta_2 \sim$ independent Uniform(0,1), then choose to be

parents the current generation members i_1^* and i_2^*, where

$$i_1^* = \min\left\{ i : \sum_{j=1}^{i} \psi_j \geq \zeta_1 \right\} \qquad \text{and} \qquad i_2^* = \min\left\{ i : \sum_{j=1}^{i} \psi_j \geq \zeta_2 \right\}.$$

- With probability $1 - P_{crossover}$, the child is identical to the modified parent if it has the larger original fitness level. (We used $1 - P_{crossover} = 0.1$.)
- With probability $P_{crossover}$, the parents with artificial implantation both contribute towards the child, in the following manner. Each member of the current generation can be represented by a vector of $N - n$ zeros and n ones, with a one indicating that the corresponding unit is included in the sample. The two vectors arising from the parents are summed, resulting in a vector with elements in $\{0, 1, 2\}$. The sum vector is adjusted to have exactly n_h non-zero elements in each h^{th} strata by randomly (uniformly) choosing an appropriate number of the ones and replacing them by zeros. Any twos are changed to ones (which means that any points common to both parents are retained). The child formed in this way is added to the new generation.
- Mutation is applied independently n times to each child - regardless of how the child is formed - as follows. For each mutation, randomly choose a one and a zero in the same stratum. Then, with probability $P_{mutation}$, swap the zero and the one and with probability $1 - P_{mutation}$ do nothing. (We used $P_{mutation} = 0.05$.)

The procedure is repeated until n_g members of the new generation are formed.

4. Step 3 is carried out until the next generation has been formed. Then its fitness levels are computed and the process is repeated from Step 2. The loss is guaranteed to decrease (weakly) in each generation, because of the inclusion of the elite members. We run the algorithm until the best design has not changed in 200 consecutive generations.

In the following, with Step 3 (b) **AI,** the algorithm is called the modified genetic algorithm with **AI**. Otherwise, it is called the modified genetic algorithm without **AI**. We will use the modified genetic algorithm with **AI** to find the optimal robust design for the sugar farm population and the MU281 population in the following two sections. In the last section, we will use the sugar farm population to compare the modified genetic algorithms with/without **AI**. We will see that the modified genetic algorithm with **AI** does run faster than the modified genetic algorithm without **AI**. This means that the modified genetic algorithm with **AI** will converge to the corresponding minimum loss in fewer generations than the modified genetic algorithm without **AI.**

4.3 The sugar farm population

We consider the sugar farm population (Chambers and Dunstan 1986) to apply our design methodology in a small but realistic population. This population consists of

Figure 4.1: Minimum loss vs. generation Case 1 of sugar farm when $g_0(x) = x, \delta = 0.15$

Table 4.1. Components of minimum loss for Case 1 of sugar farm when $g_0(x) = x$.

	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

$N = 338$ 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.

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

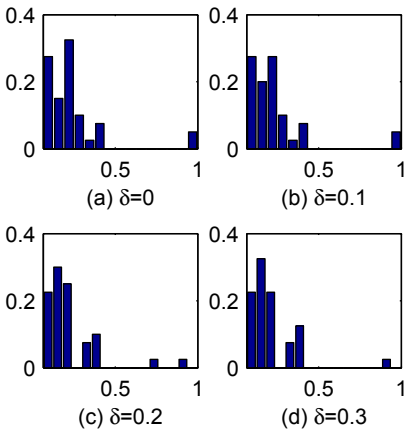

Figure 4.2: Robust designs for Case 1 of sugar farm when $g_0(x) = x^3$ and $\delta = 0, 0.1, 0.2, 0.3$

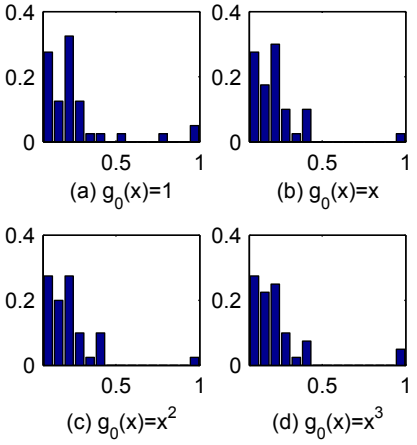

Figure 4.3: Robust designs for Case 1 of sugar farm when $\delta = 0.15$ and $g_0(x) = 1, x, x^2, x^3$

Table 4.2. Components of minimum loss for Case 1 of sugar farm when $g_0(x) = x^2$.

	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

Table 4.3. Components of minimum loss for Case 1 of sugar farm when $g_0(x) = x^3$.

	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

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 (2.1) 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 4.3 (b). From Figure 4.1, 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 4.2, the designs for different values of δ are represented as histograms. To see the effect of $g_0(x)$ on the design, in Fig 4.3, we draw the histograms corresponding 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 4.1 for $g_0(x) = x$, Table 4.2 for $g_0(x) = x^2$ and Table 4.3 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. $N_1 = 70$, $N_2 = 63$, $N_3 = 98$, $N_4 = 49$, $N_5 = 28$, $N_6 = 30$.

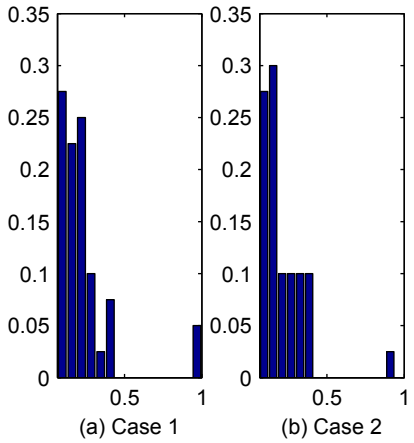

Figure 4.4: Robust designs for Cases 1 and 2 of sugar farm when $g_0(x) = x^3, \delta = 0.15$

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 4.4.

The components of the loss for the optimal design for different values of δ are shown in Table 4.4 for $g_0(x) = x$, Table 4.5 for $g_0(x) = x^2$ and Table 4.6 for $g_0(x) = x^3$. Comparing Table 4.1 with Table 4.4, Table 4.2 with Table 4.5, and Table 4.3 with Table 4.6, we observe that the minimum loss depends heavily on the initial distribution

Table 4.4. Components of minimum loss for Case 2 of sugar farm when $g_0(x) = x$.

	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 4.5. Components of minimum loss for Case 2 of sugar farm when $g_0(x) = x^2$.

	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

$F_0(x)$.

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

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

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 4.7. In the second row of Table 4.7, we list the minimum loss corresponding to robust designs. We can observe that robust designs give us smaller loss than non-robust designs.

Table 4.6. Components of minimum loss for Case 2 of sugar farm when $g_0(x) = x^3$.

	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 4.7. Comparison of robust/non-robust designs for sugar farm when $g_0(x) = x$.

	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

4.4 MU281 population

We consider the MU281 population (Särndal, Swensson and Wretman 1992) to apply our optimal design methodology in a small but realistic population. This population consists of $N = 281$ all municipalities but Stockholm, Göteborg and Malmö in Sweden. The population has an auxiliary variable $REV84$ which is the real estate value (in millions of kronor) according to 1984 assessment on each municipality. Assume that, based on the auxiliary variable $REV84$, the population is divided into $L = 4$ strata with sizes $N_h, h = 1, \cdots, L$. 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 $(N_1/N, N_2/N, N_3/N, N_4/N)$ of four strata as the $\mathbf{p}^0$ of the strata under the working distribution $F_0(x)$. We run the modified genetic algorithm with **AI** in the following two cases:

Case 1. $N_1 = 127$, $N_2 = 79$, $N_3 = 46$, $N_4 = 29$.

So, the strata sample sizes are $n_1 = 18$, $n_2 = 11$, $n_3 = 7$, $n_4 = 4$ and $\mathbf{p}^0 =$

Table 4.8. Components of minimum loss for Case 1 of MU281 when $g_0(x) = x$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$L_{0,\delta}$	4.02	5.346	7.194	9.564	12.454	15.859	19.782	24.215	29.146
L_v	0.173	0.173	0.173	0.174	0.174	0.175	0.175	0.175	0.176
$\mathcal{L}$	4.193	5.519	7.367	9.738	12.628	16.034	19.957	24.39	29.322

$(127/281, 79/281, 46/281, 29/281)'$. We ran the modified genetic algorithm with **AI** to find optimal robust designs for the working distribution and variance function in (2.1) with $g_0(x) = x$ and $\delta = 0.15$. We find that the minimum loss is 9.738. For the robust design, the sampled covariates, in the original scale, are

$$\{347, 359, 422, 1457, 1462, 1470, 1491, 1500, 1508, 1509, 1515, 1544, 1592, 1606,$$
$$1610, 1622, 1626, 1630, 1645, 1652, 1670, 2898, 2903(2), 2914, 2955, 3053, 3065,$$
$$3073, 3096, 3252, 3264, 3281, 3298, 3307, 6087, 6317, 6382, 6389, 13205\}.$$

The corresponding design is represented as a histogram in Fig 4.5 (b). From Fig 4.5 (a), we can see that the loss decreases for roughly the first 100 generations and then is fairly stable; the algorithm terminated in fewer than 500 generations.

The components of the loss for the optimal design for different values of δ are shown in Table 4.8 for $g_0(x) = x$, Table 4.9 for $g_0(x) = x^2$ and Table 4.10 for $g_0(x) = x^3$. From Tables 4.8, 4.9 and 4.10, we can observe that L_δ is increasing in δ. Moreover, each component of the minimum loss depends on $g_0(x)$.

Case 2. $N_1 = 120$, $N_2 = 86$, $N_3 = 44$, $N_4 = 31$.

Table 4.9. Components of minimum loss for Case 1 of MU281 when $g_0(x) = x^2$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$L_{0,\delta}$	1.384	2.368	3.699	5.37	7.3.71	9.704	12.365	15.354	18.671
L_v	0.061	0.061	0.061	0.062	0.062	0.062	0.063	0.063	0.063
$\mathcal{L}$	1.445	2.429	3.76	5.432	7.433	9.766	12.428	15.417	18.734

Table 4.10. Components of minimum loss for Case 1 of MU281 when $g_0(x) = x^3$.

	δ								
Loss	0	.05	.10	.15	.20	.25	.30	.35	.40
$L_{0,\delta}$	0.735	1.379	2.238	3.307	4.591	6.087	7.796	9.718	11.853
L_v	0.031	0.031	0.031	0.032	0.032	0.032	0.032	0.032	0.032
$\mathcal{L}$	0.766	1.410	2.269	3.339	4.623	6.119	7.828	9.750	11.885

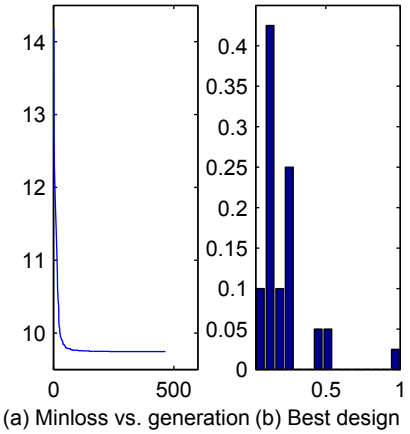

Figure 4.5: Minimum loss vs. generation and best design for Case 1 of MU281 when g(x)=x and $\delta = 0.15$

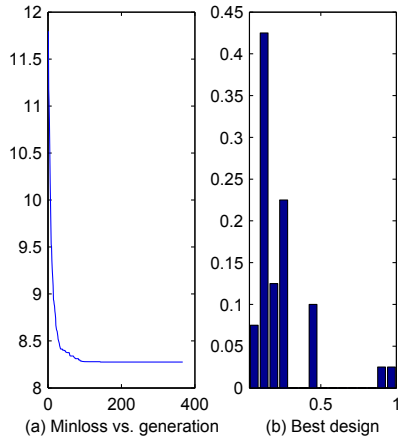

Figure 4.6: Minimum loss vs. generation and best design for Case 2 of MU281 when g(x)=x and $\delta = 0.15$

To see the effect of the initial distribution $F_0(x)$, we take $N_1 = 120$, $N_2 = 86$, $N_3 = 44$, $N_4 = 31$. Then with $g_0(x) = x$ and $\delta = 0.15$, we find that the minimum loss is 8.279. In Case 1 and Case 2, the distance between the corresponding P^0 is 0.036639 but the change of minimum loss is 1.459 which is relatively large.

For the robust design, the sampled covariates, in the original scale, are

$$x = \left\{ \begin{array}{c} 347, 359, 422, 1387, 1416, 1438, 1444, 1447, 1457, 1460, 1462, 1470, 1491, 1500 \\ 1508, 1509, 1515, 1544, 1592, 1606, 2836, 2898, 2903, 2903, 2914, 2955, 3053, 3065, \\ 3073, 3096, 3252, 3264, 3281, 3298, 6050, 6067, 6087, 6317, 12112, 13205, \end{array} \right\}$$

which are significant differ from the sampled covariates obtained in Case 1:

$$x = \left\{ \begin{array}{c} 347, 359, 422, 1457, 1462, 1470, 1491, 1500, 1508, 1509, 1515, 1544, 1592, 1606, \\ 1610, 1622, 1626, 1630, 1645, 1652, 1670, 2898, 2903(2), 2914, 2955, 3053, 3065, \\ 3073, 3096, 3252, 3264, 3281, 3298, 3307, 6087, 6317, 6382, 6389, 13205. \end{array} \right\}$$

The corresponding design is represented as a histogram in Fig 4.6 (b). From Fig 4.6 (a), 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.

4.5 Comparison of the modified genetic algorithm with/without artificial implantation

In this section, we use the sugar farm population to compare the modified genetic algorithm with **AI** and the modified genetic algorithm without **AI**. For the sugar farm population in Case 1, when $g(x) = x$ and $\delta = 0.25$, we ran each of these two algorithms 100 times. We obtain the minimum losses and the numbers of generation required to converge to the corresponding minimum loss. In the following figures and graphs, **AI**=0 denotes the modified genetic algorithm without **AI**, **AI**=1 denotes the modified genetic algorithm with **AI**.

To compare the minimum losses for these two algorithms, we get the summary statistics of the minimum losses in Table 4.11, percentiles of the minimum losses in Table 4.12 and the boxplot of the minimum losses in Fig 4.7. We find that two algorithms would give us roughly the same minimum loss. According to the result of two sample t-test in Table 4.13, we do not have strong confidence to conclude that two algorithms give us different minimum losses.

To compare the convergence speed of these two algorithms, we obtain summary statistics of generations in Table 4.14, percentiles of generations in Table 4.15, the

Table 4.11. Summary statistics for minimum losses

AI	Min	$Q1$	Median	$Q3$	Max	Mean	Std
1	33.0796	33.0796	33.0820	33.0850	33.1404	33.0842	0.0098
0	33.0796	33.0796	33.0820	33.0837	33.1410	33.0835	0.0091

Table 4.12. Percentiles of minimum losss

AI	10	20	30	40	50	60	70	80	90
1	33.0796	33.0796	33.0796	33.0796	33.082	33.082	33.0825	33.085	33.0915
0	33.0796	33.0796	33.0796	33.0796	33.082	33.082	33.0829	33.085	33.0877

boxplot of generations in Fig 4.8 and the separate histograms of generations in 4.9 and 4.10. It follows from Tables 4.14 & 4.15, boxplot 4.8 and histograms 4.9 & 4.10 that the modified genetic algorithm with **AI** would converge faster than the modified genetic algorithm without **AI**. To check that this is true, we do a two sample t-test. According to the result of two sample t-test in Table 4.16, we have 85% confidence to conclude that the modified genetic algorithm with AI converge faster than the modified genetic algorithm without AI.

Therefore, the modified genetic algorithm with **AI** will give us roughly the same minimum loss as the modified genetic algorithm without **AI** in less generations.

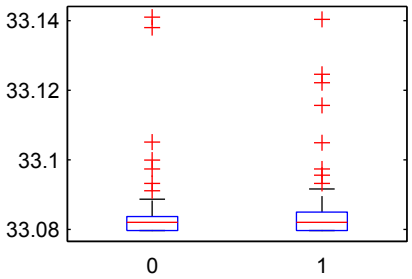

Figure 4.7: Boxplot of minimum losses without/with AI

Table 4.13. Two sample t-test for minimum loss, $\alpha = 0.01$

H_a	t-score	df	std	CI	$p-$value
$\mu_{withAI} - \mu_{withoutAI} \neq 0$	0.5161	198	0.0095	(-0.0028, 0.0042)	0.6063

Table 4.14. Summary statistics for generations

AI	Min	$Q1$	Median	$Q3$	Max	Mean	Std
1	339.000	393.500	443.500	509.000	715.000	457.960	82.841
0	298.000	391	467.5	529	852	473.51	105.348

Table 4.15. Percentiles of generations

AI	10	20	30	40	50	60	70	80	90
1	367.5	388.5	400.5	418	443.5	466.5	488	522.5	572.5
0	358	380	404.5	432	467.5	481	509	562.5	620.5

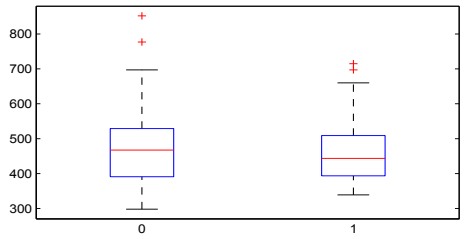

Figure 4.8: Boxplot of generations without/with AI

Table 4.16. Two sample t-test for generations, $\alpha = 0.15$

H_a	t-score	df	std	CI	$p-$value
$\mu_{withoutAI} - \mu_{withAI} > 0$	1.1603	198	94.7652	(1.6234,∞)	0.1237

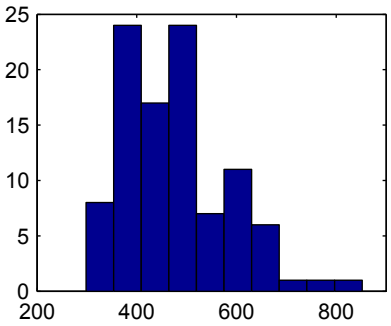

Figure 4.9: Histogram of generations without AI

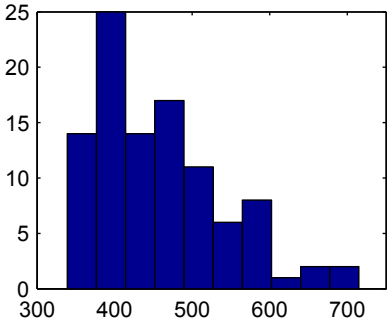

Figure 4.10: Histogram of generations with AI

Chapter 5

Conclusions and future research

In this thesis, we have studied robust sampling design for model-based stratification when the assumed distribution of an auxiliary variable x and the assumed variance function in a regression model are only approximates for true distribution and variance function. We have first obtained the mean squared error of the prediction of population total based on the regression model. Then, over the neighbourhood of the working variance function, we have found that the maximum of the mean squared error is a quadratic form in the probabilities of strata under the true distribution function. Over the neighbourhood of the working distribution, to find the maximum of the quadratic form, we have presented an analytical method which is convenient for numerical analysis. To find the robust design which minimize the maximum in the previous two stages, we have applied a modified genetic algorithm to different cases of sugar farm population and MU281 population.

In the future, we want to study on the following projects. First, we will introduce mean misspecifications in model (1.6). Secondly, we will study robust sampling

designs for cluster sampling. Thirdly, we plan to study robust sampling designs for other sampling schemes, such as two-stage sampling, multi-purposes sampling and small area sampling.

Bibliography

Bethel, J. (1989), "Minimum Variance Estimation in Stratified Sampling, " *Journal of the American Statistical Association*, *84*, 260-265.

Box, G. E. P., and Draper, N. R. (1959), "A Basis for the Selection of a Response Surface Design," *Journal of the American Statistical Association*, **54**, 622-654.

Chambers, R. L., Clark, R. G. (2012), *An Introduction to Model-based Survey Sampling with Applications*, Oxford: Oxford University Press.

Chambers, R. L., and Dunstan, R. (1986), "Estimating distribution functions from survey data," *Biometrika*, **73**, 597 - 604.

Daemi, M., and Wiens, D. P. (2012), "Techniques for the construction of robust regression designs," *The Canadian Journal of Statistics*, **41**, 679-695.

Dalenius, T. (1950), "The problem of optimum stratification," *Scandinavian Actuarial Journal,* **3-4**, 203–213.

Dalenius, T., and Hodges, J. L. (1959), "Minimum variance stratification," *Journal of American Statistical Association*, **54**, 88-101.

Fang, Z., and Wiens, D. P. (2000), "Integer-valued, minimax robust designs for estimation and extrapolation in heteroscedastic, approximately linear models," *Journal of the American Statistical Association*, **95**, 807-818.

Ghosh, S. P. (1963), "Optimum stratification with two characters," *The Annals of Mathematical Statistics*, **34**, 866-872.

Godfrey, J., Roshwalb, A,, and Wright, R. L. (1984). "Model-Based Stratification in Inventory Cost Estimation," *Journal of Business & Economic Statistics,* **2**, 1-9.

Hager, W. W. (2001), "Minimizing a quadratic over a sphere," SIAM Journal on Optimization, **12**, 188-208.

Heo, G., Schmuland, B. and Wiens, D. P. (2001), "Restricted minimax robust designs for misspecified regression models," *The Canadian Journal of Statistics*, **29**, 117-128.

Horgan, J. (2006), "Stratification of skewed populations: A review," *International Statistical Review,* **74**, 67–76.

Huber, P. J. (1981), "Robust Statistics," Wiley.

Kott P. S. (1985) "A Note on Model-Based Stratification, ," *Journal of Business & Economic Statistics,* **3**,284-286.

Li, K. C. (1984), "Robust regression designs when the design space consists of finitely many points," *The Annals of Statistics*, **12**, 269-282.

Li, K. C., and Notz, W. (1982, "Robust designs for nearly linear regression," *Journal of Statistical Planning and Inference*, **6**, 135-151.

Marcus, M. B., and Sacks, J. (1976), "Robust designs for regression problems,.in: Statistical Decision Theory and Related Topics II," ed. S. S. Gupta and D. S. Moore, New York: Academic press, pp. 245-268.

Pesotchinsky, L. (1982); "Optimal robust designs: linear regression in $\mathbb{R}^k$," *The Annals of Statistics*, **10**, 511-525.

Sorensen, D. C. (1982) , "Newton's method with a model trust region modification," *SIAM Journal on Numerical Analysis*, **19,** 409-426.

Valliant, R., Dorfman, A. H., and Royall, R. M. (2000), *Finite Population Sampling and Inference – A Prediction Approach*, Wiley.

Rockafellar, R. T. (1970), *Convex Analysis. Princeton*, N.J.: Princeton Univ. Press.

Säarndal, C. E., Swensson, B. and Wretman, J. (1992), *Model Assisted Survey Sampling. Springer-Verlag*, New York.

Sacks, J., and Ylvisaker, D. (1978), "Linear estimation for approximately linear models," *The Annals of Statistics*, **6**, 1122-1137.

Shi, P., Ye, J. and Zhou, J. (2003), "Minimax robust designs for misspecified regression models," *The Canadian Journal of Statistics*, **31**, 397-414.

Welsh, A. H. and Wiens, D. P. (2013), "Robust model-based sampling designs," *Statistics and Computing*, **23**, 689-701.

Wiens, D. P. (1990), "Robust, minimax designs for multiple linear regression," *Linear Algebra and Its Applications*, **127**, 327-340.

Wiens, D. P. (1992); "Minimax designs for approximately linear regression," *Journal of Statistical Planning and Inference*, **31**, 353-371.

Wiens, D. P. (2014); "Robustness of Design," a chapter of an upcoming Handbook of Design and Analysis of Experiments, Chapman & Hall/CRC. In press.

Wiens, D. P., and Xu, X. (2008), "Robust prediction and extrapolation designs for misspecified generalized linear regression models," *Journal of Statistical Planning and Inference*, **138**, 30-46.