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# Examination of approaches to calibration in survey sampling

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# Summary

The analysis of sample surveys is one of the key areas in official statistics. An integral part of analysing sample data is choosing appropriate weights for each sample member. These weights can informally be thought of as the number of population members each person in the sample represents.

Calibration is a method that adjusts the weights assigned to sample members in order to satisfy (or approximately satisfy) some pre-determined constraints. These are typically based on Census data or other large surveys. The key idea is that estimates formed from the weighted sample should replicate the known values from other sources.

This thesis begins with the mathematical formulation of the calibration problem as an optimization problem. Whilst the calibration problem has been defined in existing calibration literature, it has not been clearly formulated as a problem in optimization. New calibration functions are also presented, and an outline of their benefits compared to existing calibration functions given.

Much of the calibration literature focuses on so-called hard calibration. This requires an exact matching between the weighted sample data and the pre-determined constraints. However, relaxing this condition can often lead to more "well-behaved" solutions. This is the idea behind soft calibration, which has received less attention in existing literature. In this thesis, soft calibration is formulated using an optimization framework, and also presented as a diagnostic tool for identifying problematic constraints.

For many practitioners, the variance (and mean square error) of the estimates obtained is of particular interest. This is the motivation for a new approach to calibration that seeks to directly minimize the mean square error of the calibration estimator. This method is compared with existing calibration techniques, and future research directions for this approach are considered.

# Declaration

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This thesis is being submitted in partial fulfilment of the requirements for the degree of PhD.

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This thesis is the result of my own independent work/investigation, except where otherwise stated. Other sources are acknowledged by explicit references. The views expressed are my own.

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# Publications and Presentations

## Publications

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## Awards

- Best Presentation at RSC Conference 2016, University College Dublin.
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- Best Presentation at YSM 2015, Cardiff University.
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## Presentations

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- G. P. Davies, J.W. Gillard, and A. A. Zhigljavsky. Calibration in Survey Sampling. *Young Statisticians' Meeting, University of Bristol.* July 2014.

- G. P. Davies, J.W. Gillard, and A. A. Zhigljavsky. Calibration in Survey Sampling. *ONS Seminar Series, Office for National Statistics, Newport.* May 2014.

- G. P. Davies, J.W. Gillard, and A. A. Zhigljavsky. Calibration in Survey Sampling. *RSC Conference, University of Nottingham.* April 2014.

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- G. P. Davies, J. W. Gillard, and A. A. Zhigljavsky. Calibration in Survey Sampling. *Statistics and Operational Research Seminar Series, Cardiff School of Mathematics.* November 2013.

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# 1 Introduction

Calibration is a methodology for improving the estimates from survey samples, and is used by many statistical offices throughout the world. It is one of the key issues in official statistics and analysis of panel data (in particular, in market research). The Office for National Statistics [42], Statistics Belgium [62], Statistics Canada [22] and Statistics Netherlands [40] are just some of the major national statistical offices that use the method of calibration.

The work in this thesis considers the calibration problem and its use in producing estimates from survey samples. The calibration problem is formulated in terms of an optimization problem, and several new calibration functions are introduced. The motivation for and benefit of these functions shall be considered. So-called soft calibration is then explored and its use both as a calibration and diagnostic tool investigated. Finally, a new approach to calibration is proposed that minimizes the mean square error of the calibration estimator.

In this chapter, the motivation for the calibration problem is outlined and a brief overview of existing methodologies given. The main contributions of this work are presented, and an outline of the remaining chapters given.

## 1.1 The Calibration Problem

In the analysis of survey samples, members of the sample are assigned a number, most commonly referred to as a 'sampling weight'. Informally, this weight can be thought of as how many people in the population the sample member represents. Calibration is a technique that adjusts these sample weights with the aim of improving estimates.

To adjust the sample weights, additional information is used. Based upon Census data, or other large surveys, it is often possible to know the population total, mean or proportion for other variables measured in the survey, as well as the values recorded for the members of the sample. Typical examples include the proportion of males and females, the mean number of bedrooms in a household,

or total income. The variables for which this additional information is known are referred to as auxiliary variables.

The mathematical problem of calibration can be defined informally as follows. Suppose there are some initial weights (often referred to as design weights) $d_1, ..., d_n$ assigned to $n$ objects of a survey. Suppose further that there are $m$ auxiliary variables and that for these auxiliary variables the sample values are known, either exactly or approximately. The calibration problem seeks to improve the initial weights by finding new weights $w_1, ..., w_n$ that incorporate the auxiliary information. In a typical practical problem, the sample size $n$ is rather large (samples of order $10^4$ and larger are common). The number of auxiliary variables $m$ can also be large although it is usually much smaller than $n$.

Many of the developments in classical statistics are *model-based*, i.e. they rely on a specific underlying probability model that describes the random process to generate the data. There are many possible choices for this model. It could be a relatively simple model, such as a Normal distribution, or a more complicated model that involves several variables and incorporates the inter-dependence between data values. Since we consider the model as a process for generating the data, it is possible to make conclusions that can be generalized to other data generated using the same process. However, a model can only ever approximate the true data. It is often difficult to truly know how deviations from the model will affect the analysis.

However, the analysis of sample surveys is usually *design-based*. In this case, the population is pre-specified. Data values for the population are considered to be fixed, rather than random. In the design-based setting, the observed sample is considered to be random, since the sample is generated by selecting individuals at random from the fixed population. Since the random selection of individuals, referred to as the sample design, can be controlled, the probabilities of selecting individuals can often be known exactly. The analysis of the sample survey is to estimate features of the fixed population. In the design-based framework, one cannot generalize the results of the inference to other populations.

One of the important concepts for design-based methods is that of a probability sample. There is an important distinction to be made between taking a "random sample of 100 people" versus taking a "simple random sample of 100 people". In the latter, any subset of 100 people from the population is equally likely to be selected. However, there are other methods for selecting random samples, which include stratified sampling, cluster sampling, probability proportional to size sampling, to name a few. The initial weights used in calibration are typically derived using one of the standard survey sampling techniques. A brief description of each of these sampling methods is given below.

*Simple Random Sampling* In this case, each member of the sample is considered equally likely to be selected. This is one of the most elementary ways of considering members of a sample, however further results based on this approach are generally simple to derive. The design weights are simply taken to be $N/n$, where $N$ is the population size and $n$ is the sample size.

*Stratified Sampling* In stratified sampling, the population is divided into strata. These are typically based on regions or specific sections of the population. For example, counties in the UK could be considered suitable strata for a survey. Samples are then selected according to the relevant size of each strata. Suppose there are $h$ strata. Let $n_h$ denote the number of sample members of stratum $h$, and $N_h$ denote the number of population members in this stratum. Then the design weight for sample members from stratum $h$ will be $\frac{N_h}{n_h}$.

*Cluster Sampling* A drawback of stratified sampling is that it requires sample members to be drawn from each stratum. This is practically time consuming and can come with a high cost. For example, consider the example of UK counties. Under stratified sampling, sample members from each UK county would need to be sampled. A simpler approach is to select counties at random, and then either survey everyone in that county (one-stage cluster sampling) or select a random sample of people from each cluster (two-phase cluster sampling). For both one-stage and two-stage cluster sampling, design weights can be derived for the sample members. The mathematical formulation is not considered here to avoid the use of cumbersome and irrelevant notation.

For the remainder of this thesis, the design weights shall be assumed known and already derived. Lohr in [34] provides a more detailed discussion of these sampling methods and outlines many other types of sampling methods.

In practice, the initial weights are often designed to account for non-response, selection bias and other typical sampling errors. Statistical offices invest time in ensuring the initial weights are chosen appropriately to account for any biases and errors in the survey. Therefore, the initial weights have an important practical significance. It is thus desirable not to deviate too far away from these weights. This is a standard requirement in calibration, i.e. the calibrated weights should remain close to the initial weights, whilst at the same time accounting for new information gained through the auxiliary variables.

## 1.2 Motivation

According to Särndal in [51], there are six main motivations and uses for calibration in practice. In this section, each of these motivations are outlined. Further motivations and uses for calibration are also discussed.

Firstly, calibration can be used as a linear weighting method. National statistical offices often use weighting methods, and this is the main motivation behind the calibration methodology. Assigning an appropriate weight to each sample member and then considering a weighted sum of the variable values to form estimates is now a standard procedure, especially in the estimation of totals and means. Furthermore, weighting is relatively simple to explain to users of the data and stakeholders of the statistical offices.

Secondly, calibration can be thought of as a systematic way to use auxiliary information. Auxiliary information has been used to improve accuracy in survey estimation for a long time, well before the term calibration was even coined. As argued by Rueda, Martinez, Martinez and Arcos in [49], calibration is a simple and practical way of including auxiliary information as part of the estimation process.

The third use of calibration is to achieve consistency. This has already been considered in the previous section. Calibration is a method of obtaining consistent estimates with known totals. Calibration imposes constraints on the weights to ensure that weighted sample estimates replicate known population totals.

Credibility is often called into question when estimates of population quantities do not agree. For example, consider a statistical office that publishes Census data, from which the proportion of males aged 16-25 living in a particular region of the UK is known. However, the statistical office then conducts a survey and assigns design weights to members of the sample. It is possible that the estimated proportion from the sample based on these design weights will not match the known population proportion from the Census data. This leads to a contradiction in the statistics published via two data sources, which draws into question the validity of the statistics.

Fourthly, calibration offers convenience and transparency as a method. It is relatively easy to interpret the resulting estimates, and the method is easy to motivate since it is based on design weights and natural calibration constraints.

The final two points for consideration are that calibration can be used in combination with other terms and developed to give new directions of thought. Calibration will be combined with the term mean square error as a new direction of thought presented in Chapter 6. Examples of existing methods that combine calibration with other terms include model calibration [63], g-calibration [62], and regression calibration [18]. These shall be described further in Section 1.4.

The paper of Beaumont and Bocci, [8], provides further motivations for the calibration problem. They motivate calibration as a method for reducing the sampling variance of estimates. Informally, the inclusion of the additional auxiliary variables can lead to a reduction in the variance of the estimators [37]. In Chapter 6, a calibration method is considered that guarantees an estimator with minimal sampling mean square error.

Calibration can be used to reduce the sampling errors made during the survey collection process [8]. Whilst these are often accounted for when producing the

initial weights, calibration can further help to account for biases such as under-representation of certain sections of the population or non-response bias.

Many authors account for non-response bias through imputation or weighting. Calibration plays a role in the weighting approach to dealing with non-response. For example, Kott in [32] and Lundström in [37] describe how to adjust for non-response and sampling errors through an amendment to the calibration weighting methodology. This is an interesting area for future research but shall not receive further consideration in this thesis.

## 1.3 Practical Considerations

The literature on calibration is extensive, with a vast array of authors proposing methods and approaches to solving the calibration problem. However, lots of the literature on calibration is highly theoretical and difficult to implement in practice. Statistical offices are interested in using methods that can be routinely applied and that are relatively simple for all data users to understand. Therefore, only a small selection of existing calibration methods are implemented. Several of the existing calibration methods are described in Section 1.4.

Another practical consideration is whether the calibration problem can be solved. Depending on the nature of the calibration constraints, it may not be possible to find a solution to the calibration problem. This is not desirable in practice, as statistical offices require a methodology that can be used for several datasets. For example, the Labour Force Survey conducted by the Office for National Statistics is a quarterly survey. Calibration is performed on each of the quarterly datasets, each having their own calibration constraints. Therefore, a method that is adaptable and guaranteed to give a solution is highly desirable.

However, even methods that are guaranteed to give a solution to the calibration problem may result in weights that are practically unappealing. Negative weights may occur for certain calibration methods. Using the informal definition of a weight as the number of population members represented, negative weights would

suggest that the sample member does not account for anyone in the population, even themselves.

Similarly, very large weights are undesirable in practice, since this leads to certain members of the sample dominating the results. Whilst certain sample members may be considered "more representative" than others, sample members should all contribute to the population estimates. Large calibration weights are often observed with small calibration weights for other sample members. Those with large weights are typically over-represented, whilst those with small weights are under-represented in the survey.

In this thesis, these practical considerations are explored and approaches for dealing with the undesirable effects discussed. The use of calibration functions, range restrictions and soft calibration are considered for dealing with negative and large weights. The use of soft calibration as a diagnostic tool in the case of calibration problems with no solutions is also presented.

## 1.4 Classical Literature

In this section, several existing calibration methodologies and approaches are considered. The two main types of calibration are introduced and their benefits and drawbacks explored. The first of these, hard calibration, imposes a strict condition on the auxiliary variables. The constraints used to obtain the calibrated weights are required to be satisfied exactly. However, this can lead to undesirable effects such as negative weights and extreme weights. In contrast, soft calibration relaxes this condition slightly with the aim of finding solutions that are more "well-behaved".

Calibration is a key method in official statistics, and there is a great field of literature in this area. It forms an important part of the analysis of sample surveys, with the aim of improving estimates by using existing information. Calibration has already been introduced as a method of improving estimates through the use of auxiliary variables. For these auxiliary variables, the population totals as well

as the sample values are known. This may be through Census data or via other large surveys.

There is an extensive literature on calibration, with many authors extending and proposing alternative methods. It would be impossible for this thesis to acknowledge all the areas of calibration outlined in existing literature. Instead, the discussion in this chapter focuses on the methodologies that are implemented in practice and have relevance to the work described throughout this thesis.

It can be argued that the term 'calibration' was first introduced by Deville and Särndal in the classical paper [19]. These authors were the first to coin the term 'calibration', and presented the most standard approach to calibration used to this day. The material introduced in this paper forms the basis for most of the calibration performed in statistical offices throughout the world.

However, that is not to say that the idea of calibration did not exist before this. Weighting methods similar to calibration have been used by statistical offices for many years. Weighting observed sample values has been an important area of research in official statistics for many years. For example, Alexander in [1] uses the terminology "household weighting" and "constrained minimum distance". The methodology is essentially equivalent to the calibration problem that will be presented in Chapter 2. Similarly, Bethlehem in [7] describes the use of linear weighting and regression estimation to derive a weighted estimate that is equivalent to a calibration estimator.

This section is dedicated to the literature on hard calibration, as well as its use in many statistical offices throughout the world. The existing research in the area of soft calibration is then explored and a brief overview of the current methodologies is given.

There are many algorithms and statistical software packages used for performing calibration. These are not considered in this section. A more detailed explanation of the algorithms and software used by statistical offices to perform calibration is given in Chapter 3.

### 1.4.1 Hard Calibration

Almost all the research in calibration references the classical paper 'Calibration Estimators in Survey Sampling' of Deville and Särndal [19]. Whilst weighting methods and the idea of calibration existed long before the work presented in this paper, the term 'calibration' was first coined by these authors and their method remains the most standard approach to calibration.

The material introduced by these Deville and Särndal forms the basis for most of the calibration performed in statistical offices throughout the world. Calibration is presented as a methodology for finding alternative sample weights that are as close as possible to some pre-determined initial weights, whilst satisfying the so-called hard calibration equation. This hard calibration equation uses auxiliary variables, for which sample values and population totals are known. This additional information typically comes from Census and other survey data. The key calibration idea is finding new calibration weights that are as close as possible to the initial weights, whilst satisfying the calibration equation.

Särndal in [51] reiterates the importance of calibration as a method for including auxiliary information as part of the estimation process, and that the thought process for calibration is different to that for regression and generalised regression estimation presented by Särndal, Swensson and Wretman in [52].

Särndal continues in [51] to suggest that no pre-determined specification of a model is required, instead the emphasis is on how the auxiliary information can be used to improve estimates. In contrast, generalized regression estimation focuses on the use of a so-called assisting regression model to improve estimates. A more detailed overview of generalized regression estimation is given by Fuller in [24].

Based on the purpose of the calibration, Särndal in [51] suggests alternative names for the calibration approach. Recall that one use of calibration is consistency with known totals, often referred to as controls. In this case, the term "controlled weighting" is often used, which also reflects the improved accuracy in the estimation. The French term for calibration, "calage", also refers to the notion of stability and consistency.

However, when the motivation for calibration is primarily a reduction in variance and/or the non-response bias, the phrase "balanced weighting" is considered more appropriate. This thesis introduces the term mean square error calibration in Chapter 6, which arguably belongs to the class of "balanced weighting" methods.

A further extension of calibration has been to so-called "repeated weighting" calibration. As the name suggests, in this approach the calibration weighting method is repeated several times. The motivation for this approach is to obtain consistency with variables from different surveys. Similarly, if the same variables are considered in two or more surveys, then there is practical appeal in ensuring that the weighted estimates from both surveys produce the same estimate of the unknown population parameter. The work of Renssen in [48] considers aligning estimates for common variables from two or more surveys, whilst Renssen in [47] considers repeating the weighting several times to ensure consistency of the survey estimates.

In Section 1.2, it was stated that calibration is often used in combination with other terms as a new direction of thought. Since the classical paper by Deville and Särndal [19], there has been extensive research and further developments of the calibration problem. It would be impossible to consider all the areas of research, but a summary of some of the key methods is given in this section. The reader is referred to the paper of Särndal [51] for a more extensive review of the developments in calibration methods.

Model calibration is presented by Wu and Sitter in [63]. In this approach, an explicit model is used to relate the variable of interest and the auxiliary variables. The term 'model-assisted' is also used by these authors, since it can be argued that the model is used to assist the calibration process. Inevitably, this approach relies on the suitability of the model. The use of models with calibration shall be considered further in Chapter 6.

Another term used is $g$-calibration. Essentially, this approach solves calibration through the use of $g$-weights, which are defined to be the ratio of the calibrated and initial weights, i.e. $g_k = \frac{w_k}{d_k}$, where $g_k$ denotes the $g$-weight for the $k$-th sample member ($k = 1, \ldots, n$), whilst $w_k$ and $d_k$ denote the calibrated and initial weights

respectively. The paper of Deville, Särndal and Sautory in [20] presents much of the work from Deville and Särndal's paper of [19] using $g$-weights. The term $g$-calibration is also used by Vanderhoeft in [62].

Regression calibration is also a term considered by Demnati and Rao in [18]. This is arguably a more specific case of model calibration, where regression models are used to describe the relationship between the variable of interest and auxiliary variables. The authors consider various types of regression models, including linear regression, multiple regression and logistic regression.

A further use of calibration has been as a method of adjusting imputed missing values. Instead of adjusting sample weights to satisfy pre-determined constraints, the imputed sample values are themselves adjusted to satisfy several constraints. This method aims to account for the biases and errors that can occur through imputation methods. The theory is very similar to that of adjusting weights in the standard approach to calibration.

For the purposes of this thesis, calibration is considered to be a method of finding new weights that are close to some pre-determined initial weights whilst satisfying some additional information. Recall that the initial weights have often been designed to account for non-response and to ensure that there is an accurate reflection of the population. To assess the 'closeness' of the initial and calibrated weights, some form of measure is required. Deville and Särndal in [19] begin by presenting a measure that is reminiscent of the chi-square statistic. The function itself is simply quadratic, and therefore the name quadratic rather than chi-square shall be used for the remainder of this thesis.

However, Deville and Särndal [19] advocate that the choice of the quadratic (chi-square) function was arbitrarily taken and suggest alternative measures. These are referred to as 'distance functions' in much of the existing calibration literature. However, not all of them satisfy the triangle inequality for distance functions. Therefore, for the remainder of this thesis, these measures will simply be referred to as calibration functions.

A drawback with the quadratic calibration function is that it can result in negative and extreme weights. The practical implications of negative and extreme

weights was outlined in Section 1.3. The drawbacks of this measure are considered throughout this thesis, particularly in Chapter 4. Alternative calibration functions presented by Deville and Särndal in [19] include one of logarithmic form. By its definition, this function cannot lead to negative weights. However it often results in calibrated weights that are extremely large compared to the initial weights. This function is often referred to as the 'raking' function, or 'raking ratio', due to its similarities to the raking ratio method developed by Deming and Stephan in [17].

The raking ratio method is arguably a pre-cursor to the existing calibration approaches. The raking ratio method adjusts sample frequencies in contingency tables to account for known expected marginal totals. The approach is very similar to the standard calibration methodology that will be considered throughout this thesis.

Three other calibration functions are proposed by Deville and Särndal [19]. The first is reminiscent of the Hellinger distance, described by Beran in [6]. The second is a minimum entropy distance, and the final one has a square root form. A solution to the calibration problem can always be found when using the quadratic and raking functions, however solutions are not guaranteed in the case of these other three functions. This is likely to explain why the quadratic and raking functions have received much more attention in subsequent calibration literature. Furthermore, only the quadratic and logarithmic functions are implemented in most survey calibration software packages. Calibration functions shall be considered in more detail in Chapter 4.

A common approach to dealing with the negative and extreme calibration weights is by imposing a restriction on the calibrated weights. In doing so, this can prevent them becoming negative or extremely large. So-called range restrictions are imposed on the calibrated weights. These are pre-determined bounds that the calibration weights must lie within. Whilst strict bounds will lead to calibration weights that are closer to the initial weights, imposing bounds that are too strict can result in the calibration problem having no solution.

Extreme and negative weights are noted by Beaumont and Bocci in [8] as motivation for weights to satisfy bounds. These bounds help control the effect of leverage points on the sampling error of estimates, as the leverage points themselves may otherwise lead to large weight adjustments. Here the term leverage points refers to extremal or outlying values that, due to their extremity, may lead to an over zealous change (or leverage) of the weights.

For the five calibration functions that have already been described, the standard approach used in algorithms is to project any weights that fall outside the bounds back to these bounds. The calibration is then performed again, with this re-scaling performed at every iteration.

However, an alternative function proposed by Deville and Särndal in [19] automatically accounts for the weight bounds. It is known as the logit function, as it is based on the logit function that is used as part of logistic regression. The benefits and drawback of this function shall be discussed throughout this thesis. In Chapter 4, two new calibration functions are proposed that are also able to give weights within desired bounds.

In this section, an overview of the existing literature in the area of hard calibration has been given. Hard calibration requires constraints on the auxiliary variables to be satisfied exactly. However, this can lead to undesirable effects such as negative weights and extreme weights. Alternative calibration functions can be used to prevent negative and extreme weights, and range restrictions can be imposed to ensure the calibrated weights do not deviate too far from the initial weights.

In the next section, a review of the existing literature for soft calibration is given. This is an alternative approach that relaxes the calibration constraints with the aim of obtaining "better behaved" solutions to the calibration problem.

### 1.4.2 Soft Calibration

In the previous section, the literature for the hard calibration problem was described. Several problems were outlined including negative weights, extreme weights and the potential for no solutions to the problem.

In this section, the literature for the soft calibration problem is presented. Unlike hard calibration, soft calibration has received much less attention in existing literature. For statistical offices, the possibility for differences between population totals and survey estimates, no matter how small, is uncomfortable from the point of view of consistency and accuracy of official statistics.

The main approach suggested in the existing literature is to borrow ideas from ridge regression in classical statistics. The term 'soft' calibration is rarely used in literature. Instead the term 'ridge calibration' is often used, for example by Beaumont and Bocci in [8]. Bardsley and Chambers in [4] consider the use of a ridge regression instead of ordinary least squares regression for deriving weighted sample estimates.

Recall that for ordinary least squares regression, one needs to invert a matrix that is made up of the auxiliary (or predictor) variables. In cases when this matrix cannot be inverted, or has a determinant that is very close to zero, the solution to the least squares regression does not exist or is very unstable. To account for this, ridge regression adds a multiple of the identity matrix to the original matrix being inverted. This multiple is often referred to as the ridge parameter. This then results in a matrix that can be inverted and gives a solution that is approximately the ordinary least squares solution.

This idea of ridge regression has been applied for calibration. In cases where a solution to the hard calibration problem cannot be found, or when the solution leads to extreme or negative weights, a ridge parameter can be used to reduce the severity of calibration constraints and lead to a more 'well-behaved' solution. This idea has been developed by Chambers [11], Rao and Singh [45] and Théberge [59]. The ridge calibration approach deals with the range restrictions by making a suitable choice of the ridge parameter, whilst at the same time trying to satisfy the calibration constraints as closely as possible. This problem shall be described in more detail in Chapter 5.

The ridge parameter is one approach to soft calibration. Another suggested by Beaumont and Bocci [8] is to relax the range restrictions until a solution is found. However, the bounds may need to be relaxed substantially until a solution is found,

contradicting the purpose of imposing the bounds. An alternative approach is to relax the calibration constraints. Examples of this come from Bankier, Rathwell and Majkowski [3], where it was proposed to drop some of the calibration constraints in the Canadian Census. Many other authors prefer a less drastic approach, only partially relaxing the calibration constraints to the point where a solution exists. Both Rao and Singh [45] and Chen, Sitter and Wu [13] propose estimators where the calibration constraints are relaxed as minimally as possible to satisfy weight bounds. This will be explored further in Chapter 5.

To relax the calibration constraints, a measure similar to the quadratic calibration function is proposed. This leads to two quadratic functions being used, the first assesses the deviation between the initial and calibrated weights, whilst the other assesses the variation of the weighted estimate from the known population totals.

Chen, Sitter and Wu in [13] propose an approach to calibration that uses empirical likelihood methods to derive a calibration estimator that satisfies range restrictions whilst approximately satisfying the calibration constraints. However, Beaumont [5] shows it's equivalence to the soft calibration problem using ridge regression and therefore for the purposes of this thesis, the method of Chen, Sitter and Wu in [13] shall not be given any further consideration.

There is a much smaller literature in the area of soft calibration, making it a more appealing area for research and further investigation. Chapter 5 is dedicated to this approach to calibration.

Whilst there are many other varieties of 'calibration' methods that have not been considered, those presented in this chapter are of greatest practical relevance and will form the basis of the content of this thesis. In the next chapter, the approaches to calibration presented in this chapter are described mathematically using an optimization framework. Chapter 3 describes the existing algorithms and software packages used to perform calibration. The choice of calibration functions shall be given further discussion in Chapter 4, including the presentation of two new calibration measures. Chapter 5 contrasts existing soft calibration methodologies to a new approach using optimization. A new approach to calibration that minimizes the mean square error of the calibration estimator will be outlined in Chapter 6.

In this section, the existing literature in the areas of hard and soft calibration has been considered. The history and developments of calibration have been outlined, and drawbacks of existing methodologies discussed. In the next section, the key contributions of this thesis will be described.

## 1.5 Main Contributions

This research considers the calibration problem in the analysis of sample surveys. This thesis will examine existing approaches to solving the calibration problem, which have lead to the development of several novel approaches proposed in this thesis. For each of the new methodologies, comparisons are made with well-known existing approaches. The following scientific contributions are made:

- Expressing calibration in terms of an optimization problem (Chapter 2).
- Mathematical formulation of the algorithms used by several existing calibration software packages (Chapter 3).
- New calibration functions that improve the behaviour of the calibrated weights and estimates (Chapter 4).
- Expressing soft calibration as an optimization problem, leading to a method that is guaranteed to have a solution independent of the 'softening' parameter used (Chapter 5).
- The use of soft calibration as a diagnostic tool in identifying problematic calibration constraints. This has the practical appeal of diagnosing problems with the calibration constraints when solutions are undesirable or cannot be found (Chapter 5).
- A new approach to calibration that directly minimizes the mean square error (MSE) of the calibration estimator. This is of practical appeal, as estimators with small variance are always desirable in practice. This approach guarantees to find the calibration estimator with minimum MSE (Chapter 6).

## 1.6 Thesis Overview

In this section, the structure of the thesis is presented and the main contributions of each chapter described.

**Chapter 2** presents the calibration problem and formulates it in terms of an optimization problem.

**Chapter 3** considers several of the algorithms and software packages that are currently used for solving the hard calibration problem. A critical analysis of these algorithms and software packages is given, with examples to illustrate their behaviour.

**Chapter 4** considers the functions that are used as part of the calibration optimization problem. Problems with existing calibration functions are outlined, and several new calibration functions are proposed.

**Chapter 5** discusses the method of soft calibration. Soft calibration is presented as an optimization problem, and its practical appeal for solving the calibration problem is explored. The use of soft calibration as a diagnostic tool for investigating problematic constraints is also discussed.

**Chapter 6** presents a new calibration methodology that minimizes the mean square error of the calibration estimator. In doing so, it finds a calibration solution whose corresponding calibration estimator has minimal MSE. This has practical appeal, since estimators with small MSE are desirable in practice.

**Chapter 7** concludes the thesis and summarises the main contributions of this research. It also provides the scope for further work and possible future areas for research.

## 1.7 Summary

In this chapter, the motivation and practical considerations for the calibration problem have been outlined. Existing literature in the areas of hard and soft

calibration has been explored. The key contributions of this research have been described, and a summary of each chapter in this thesis given.

In the next chapter, the calibration problem is introduced and defined as an optimization problem. Whilst much of the literature considered in this chapter has already described the calibration problem, none of the existing literature has clearly formulated the problem using an optimization framework. Hard and soft calibration shall both be presented as problems in optimization.

# 2 Calibration as an Optimization Problem

In this chapter, the problem of calibration of weights is formulated as an optimization problem. The motivation and practical need for the calibration problem was formulated in the previous chapter. In this chapter, the calibration problem is defined mathematically and the properties of the corresponding optimization problems outlined. Recommendations on how to choose the objective function shall be described in Chapter 4. The literature on calibration has ignored this important issue, which has lead to algorithms that were inefficient. This is discussed further in Chapter 3.

## 2.1 Introduction

In Chapter 1, the extensive literature and various directions and extension of the calibration problem were discussed. However, survey calibration can be described simply as an optimization problem. Whilst the problem is already defined in existing literature, it has not been formulated in the way presented in this chapter. This chapter provides a unified formulation of much of the work presented and described in [19] and [20].

## 2.2 Notation

Mathematically, calibration is a large-scale convex optimization problem with linear constraints. To formulate the problem, the following notation shall be used:

| | |
|---|---|
| $D = (d_1, \ldots, d_n)'$: | vector of initial weights, |
| $W = (w_1, \ldots, w_n)'$: | vector of calibrated weights, |
| $G = (g_1, \ldots, g_n)'$: | vector of the $g$-weights $g_i = w_i/d_i$ $(i = 1, \ldots, n)$, |
| $L = (l_1, \ldots, l_n)'$: | vector of lower bounds for the $g$-weights, |
| $U = (u_1, \ldots, u_n)'$: | vector of upper bounds for the $g$-weights, |
| $Y = (y_1, \ldots, y_n)'$: | vector of sample values for the variable of interest, |
| $X = (x_{ij})_{i,j=1}^{n,m}$: | given $n \times m$ matrix, |
| $A = (a_{ij})_{i,j=1}^{n,m}$: | given $n \times m$ matrix, |
| $T = (t_1, \ldots, t_m)'$: | arbitrary $m \times 1$ vector, |
| $\mathbf{1} = (1, 1, \ldots, 1)'$ | $n \times 1$ vector of ones, |
| $\mathbb{G}$ | feasible domain in the calibration problem, |
| $\mathbf{0} = (0, \ldots, 0)'$ | $n$-vector of zeros, |
| $\mathbf{1} = (1, \ldots, 1)'$ | $n$-vector of ones, |
| $I_n$ | $n \times n$ identity matrix. |

Consider the $n \times 1$ vector $Y = (y_1, \ldots, y_n)'$ of sample observations from a variable of interest. Suppose a vector of initial so-called 'design' weights $D = (d_1, \ldots, d_n)'$ is given. These initial weights are always assumed to be positive: $d_i > 0$ for all $i$. The aim is to estimate the unknown population total, denoted by $T_Y$, of the variable of interest. Given a set of sample observations and a set of initial design weights, the estimator $Y'D$ provides an estimate of the unknown population total.

The initial weights in the case of simple random sampling and stratified sampling were given in Chapter 1. The most common choice for the design weights is $d_i = \frac{1}{\pi_i}, i = 1, \ldots, n$, where $\pi_i$ denotes the inclusion probability of the $i$-th sample member. The inclusion probability is simply a measure of a sample member's likelihood of being included in the sample. In this case, the estimator $Y'D$ is called the Horvitz-Thompson estimator [28], one of the most famous estimators in survey sampling. The Horvitz-Thompson estimator is an unbiased estimator of $T_Y$.

Note, however, that whilst the estimator $Y'D$ is unbiased, the estimates it gives will vary depending on the sample taken. Any unbiased, or approximately unbiased, estimator with smaller variance than $Y'D$ would be considered a better estimator in the sense that estimates are less variable.

Calibration is a method that incorporates information from additional auxiliary variables to derive a vector of calibrated weights, $W = (w_1, \ldots, w_n)'$, from which the estimator $Y'W$ can be formed. The main objective is to obtain an estimator with improved accuracy. Unlike the Horvitz-Thompson estimator, the calibration estimator is biased. The bias of this new estimator shall be considered below.

Taking the existing literature, including [19] and [27], one can formulate the following theorem.

**Theorem 2.1** (Bias of Estimator $Y'W$)**.** *Let $D = (d_1, ..., d_n)'$ be the design weights associated with the Horvitz-Thompson estimator (therefore $d_i = \frac{1}{\pi_i}$ for all $i$). Let $W$ be a vector of calibrated weights and $Y = (y_1, \ldots, y_n)'$ be an $n \times 1$ vector of sample values of a variable of interest. Then $Y'W$ is a biased estimator of the unknown population total $T_Y$, with bias $E[Y'(W - D)]$.*

*Proof.* Combining the estimator $Y'W$ with the unbiased Horvitz-Thompson estimator, $Y'D$, gives:

$$Y'W = Y'D + Y'(W - D).$$

Hence, the bias of $Y'W$ is given by:

$$\text{bias}[Y'W] = E[Y'D + Y'(W - D)] - T_Y = E[Y'(W - D)].$$

□

It is important that the new estimator $Y'W$ is approximately unbiased for the population total. This means that $E[Y'(W - D)] \approx 0$. This suggests that calibration should strive for small deviations between $W$ and $D$. This is one of the main motivations of the calibration problem, namely that the deviations between $W$ and $D$ should be as small as possible.

To formulate the calibration problem, a method for assessing the deviations between the calibrated weights $W$ and the initial weights $D$ is required. In Chapter 1, calibration functions (referred to as 'distance measures' in the literature) were introduced as a measure for assessing the variability between the initial and calibrated weights. In Chapter 4, appropriate choices of these penalty functions

shall be discussed for quantifying the variability between the initial and calibrated weights $D$ and $W$, respectively.

## 2.3 The main constraint

Let $X = (x_{ij})_{i,j=1}^{n,m}$ be a matrix of realizations of $m$ auxiliary variables. Note that the auxiliary variables should be chosen such that they are correlated with the variable of interest introduced in Section 2.2. The $(i, j)$-th entry $x_{ij}$ of $X$ denotes the value that the $i$-th member of the sample takes on the $j$-th auxiliary variable. Formally, $X$ is an arbitrary $n \times m$ matrix. Given the vector $T = (t_1, \ldots, t_m)'$, exact (hard) constraints can be written as $X'W = T$, whereas approximate (soft) constraints are $X'W \simeq T$. These constraints, whether exact or approximate, define the additional information used in the calibration of the weights.

Often, a constraint is also given on the sum of the weights. Typically, that the sum of the weights should equal the size of the population. Recall that a sample member‘s weight can be considered as how many people in the population that person represents. This motivates the requirement that the sum of all of these weights should be the population size.

The sum of weights constraint can be written mathematically as $\sum_{i=1}^{n} w_i = N$. Alternatively, [57] formulates the constraint $\sum_{i=1}^{n} w_i = \sum_{i=1}^{n} d_i$ or, in vector notation, $\mathbf{1}'W = \mathbf{1}'D$, where $\mathbf{1} = (1, 1, \ldots, 1)'$. This is equvialent to $\sum_{i=1}^{n}$ in the majority of cases, since the initial weights are also usually taken to sum to the population total. Note that the condition $\mathbf{1}'W = \mathbf{1}'D$ can be added to the set of the main constraints $X'W = T$. Hence, the work in this thesis does not formally distinguish between the cases when the condition $\mathbf{1}'W = \mathbf{1}'D$ is required or not.

The ratios of the weights $w_i$ and $d_i$ are often considered rather than the weights $w_i$ themselves. Vanderhoeft in [62] and Deville, Särndal and Sautory in [20] consider these ratios, which they define to be so-called $g$-weights $g_i = w_i/d_i$. Several of the standard calibration packages, which shall be discussed further in Section 3.6, give $g$-weights as the output. Hence, in this chapter, the main focus will be on calibration using $g$-weights. It should be noted that some authors refer to the

values $g_i$ as calibration factors rather than calibrated weights. However, $g_i$ will be referred to as calibrated weights throughout this thesis.

Denote the vector of $g$-weights by $G = (g_1, \ldots, g_n)'$ and consider this vector as the vector of calibrated weights being sought. Since $d_i > 0$ for all $i$, the hard constraints $X'W = T$ can be written in the form $A'G = T$, where the matrix $A = (a_{ij})_{i,j=1}^{n,m}$ has elements $a_{ij} = d_i x_{ij}$. Correspondingly, soft constraints $X'W \simeq T$ have the form $A'G \simeq T$.

## 2.4 Additional constraints on the $g$-weights

There are more constraints on $G$, in addition to $A'G = T$, that must be imposed. First of all, the calibrated weights must be non-negative; that is, $g_i \geq 0$ for all $i$. Moreover, much of the calibration literature, for example Brewer in [9] and Théberge in [59], recommends imposing stricter constraints on the $g$-weights of the form $L \leq G \leq U$, where $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$ are some given $n \times 1$ vectors such that $0 \leq l_i < 1 < u_i \leq \infty$ for all $i$. That is, the $g$-weights should satisfy $l_i \leq g_i \leq u_i$ for some sets of lower and upper bounds $l_i$ and $u_i$. If $l_i = 0$ and $u_i = \infty$ for all $i$, then the constraint $l_i \leq g_i \leq u_i$ coincides with the simple non-negativity constraint $g_i \geq 0$. In the majority of practical problems, $l_i = l$ and $u_i = u$ for all $i$ with $0 \leq l < 1 < u \leq \infty$, where strict inequalities $l > 0$ and $u < \infty$ are very common.

To summarize, the three choices of the vectors $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$ are:

(a) no constraints: $l_i = -\infty$ and $u_i = \infty$ for all $i$;

(b) non-negativity constraint: $l_i = 0$ and $u_i = \infty$ for all $i$;

(c) general constraints: $0 \leq l_i < 1 < u_i \leq \infty$.

## 2.5 Problem Statement

In Section 2.2, the need for the calibrated weights $W$ to stay as close as possible to the initial weights $D$ was motivated. Equivalently, the $g$-weights $G$ have to stay as close as possible to the vector $\mathbf{1}$. To measure the "closeness" of $G$ and $\mathbf{1}$, some function $\Phi(G) = \Phi(g_1, \ldots, g_n)$ is used. This function is required to satisfy the following properties:

(I) $\Phi(G) \geq 0 \ \forall G$,

(II) $\Phi(\mathbf{1}) = 0$,

(III) $\Phi(G)$ is twice continuously differentiable, and

(IV) $\Phi(G)$ is strictly convex.

The first of these constraints requires that the function cannot be negative. We are assessing the deviation between $G$ and $\mathbf{1}$, therefore, if $\Phi(G)$ is positive, this indicates a deviation from $\mathbf{1}$. Similarly, if $G$ and $\mathbf{1}$ are the same, then the function should give zero, hence the second requirement. The twice continuously differentiable and strictly convex conditions guarantees that the calibration functions have well-behaved derivatives and have a minimum of 0 at $G = \mathbf{1}$. A more detailed discussion of these properties is given by Deville, Särndal and Sautory in [20].

The function $\Phi$ often has the form

$$\Phi(G) = \Phi(g_1, \ldots, g_n) = \sum_{i=1}^{n} q_i \phi_i(g_i)\,, \tag{1}$$

where $q_1, \ldots, q_n$ are given non-negative numbers; in the majority of applications $q_i = d_i$ for all $i$. In this chapter, the form of $\Phi$ is considered. Choices of the functions $\phi_i$ are introduced in Section 4.2.

Hard constraints $A'G = T$ enter the definition of the feasible domain of $G$. Soft constraints $A'G \simeq T$ can either enter the definition of the feasible domain of $G$ in the form $\|A'G - T\| \leq \epsilon$ for some vector norm $\|\cdot\|$ and some given $\epsilon > 0$, or can be put as a penalty $\Psi(A'G, T)$ into the objective function. The properties

required for $\Psi$ (as a function of $G$) are similar to those required for $\Phi$. The most common choice for $\Psi$ is

$$\Psi(A'G, T) = \beta^{-1}(A'G - T)'C(A'G - T) \tag{2}$$

where $C$ is some user-specified $m \times m$ positive definite (usually, diagonal) matrix and $\beta > 0$ is some constant (see for example [8], equation (2.3)).

Summarizing, there are the following versions of the calibration problem formulated in terms of the feasibility domain for the vector of $g$-weights $G$, where the function (1) plays the role of the objective function in the corresponding optimization problems.

Hard constraint case:

$$\Phi(G) \to \min_{G \in \mathbb{G}}, \text{ where } \mathbb{G} = \{G : L \leq G \leq U \text{ and } A'G = T\}. \tag{3}$$

Soft constraint case I:

$$\Phi(G) \to \min_{G \in \mathbb{G}}, \text{ where } \mathbb{G} = \{G : L \leq G \leq U \text{ and } \Psi(A'G, T) \leq 1\}. \tag{4}$$

Soft constraint case II:

$$\Phi(G) + \Psi(A'G, T) \to \min_{G \in \mathbb{G}}, \text{ where } \mathbb{G} = \{G : L \leq G \leq U\}. \tag{5}$$

In problems (3)–(5), the matrix $A$ and the vectors $T, L$ and $U$ are given, and in the majority of applications the functions $\Phi$ and $\Psi$ have the forms (1) and (26), respectively. Optimization problems (3)-(5) will be fully defined if the function $\phi$ in (1) is fully specified.

Optimization problems (3) and (4) may have no solutions, that is the feasible domain $\mathbb{G}$ in these problems may be empty. The case when $\mathbb{G}$ is empty means that the constraints on $G$ are too strong. The feasible domain $\mathbb{G}$ in problem (5) is always non-empty and the optimal solution always exists. In view of the strict

convexity of $\Phi$ and $\Psi$ as well as the compactness of $\mathbb{G}$, if the optimal solution exists then it is necessarily unique. Optimization problem (4) is difficult to implement in practice and is therefore not considered. Instead, due to the computational and practical motivations for calibration, only problems (3) and (5) shall be considered for the remainder of this thesis. These problems are generally easier to implement and computationally easier to perform. Problem (4) remains an interesting area for further research.

## 2.6 Summary

In this chapter, the calibration problem has been presented as a problem in optimization. Whilst existing calibration literature has already described the problem, it has not been clearly formulated as a problem in optimization.

This chapter began by formulating the notation required to describe the calibration problem. The main calibration constraints were described, along with additional constraints on the $g$-weights. The problem statement was then given, with three cases of optimization problems, one for hard calibration and two for soft calibration. The first formulation for soft calibration is computationally challenging, and therefore only the second shall be considered for the remainder of this thesis.

The key contribution of this chapter is the clear formulation of calibration as an optimization problem. This will form the basis of the work in many of the future chapters.

In the next chapter, several of the algorithms used for solving the hard calibration problem will be described. An outline of the key software packages that implement calibration is also given. The benefits and drawbacks of each algorithm shall be described, with practical use and run time two of the key factors.

# 3 Algorithms for Solving the Hard Calibration Problem

In this chapter, several algorithms for solving the hard calibration problem are introduced. Soft calibration is not considered in this chapter, but will be discussed in Chapter 5. The algorithms described in this chapter are used in many of the calibration software packages that are outlined in Chapter 3.6. This chapter expands on the work published in [16].

## 3.1 Introduction

Recall that the hard calibration problem is as follows:

$$\Phi(G) \to \min_{G \in \mathbb{G}}, \text{ where } \mathbb{G} = \{G : L \leq G \leq U \text{ and } A'G = T\}, \tag{6}$$

where

$$\Phi(G) = \Phi(g_1, \ldots, g_n) = \sum_{i=1}^{n} q_i \phi_i(g_i)\,. \tag{7}$$

Here $\phi$ is a specified calibration function and $q_1, \ldots, q_n$ are given non-negative numbers. In the majority of applications $q_i = d_i$ for all $i$; it is assumed that $q_i = d_i$ throughout this chapter. The vectors $L$ and $U$ are $n$-vectors of lower and upper bounds for the $g$-weights $G$, respectively, $A$ is a known matrix derived from the sample observations, and $T$ is an $m$-vector of known population totals. The three common choices of the vectors $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$:

(a) no constraints: $l_i = -\infty$ and $u_i = \infty$ for all $i$;

(b) non-negativity constraint: $l_i = 0$ and $u_i = \infty$ for all $i$; and

(c) general constraints: $0 \leq l_i < 1 < u_i \leq \infty$.

In this chapter, the following three choices of the function $\phi$ are considered. These are the standard choices for the function $\phi$ used in existing software. Other choices of the function $\phi$ shall be discussed in Chapter 4.

The first of these functions is a quadratic and commonly referred to as a chi-square measure [19]. The second is referred to as the raking function, due to its connection to the raking ratio that is used for adjusting values in contingency tables. The final function is called the logit function, based on its similarity to the logit (logistic) function. These functions are presented in terms of the $g$-weights. Since $g_i = w_i/d_i$, the functions can be re-written in terms of the calibrated weights, $w$. As $g$-weights are our main concern in this chapter, we only consider the $g$-weight forms of the functions.

(1) Quadratic:

$$\phi^{(Q)}(g) = \frac{1}{2}(g-1)^2;$$

(2) Raking:

$$\phi^{(R)}(g) = g\ln(g) - g + 1;$$

(3) Logit:

$$\phi^{(L)}(g;l,u) = \frac{1}{C}\left[(g-l)\ln\left(\frac{g-l}{1-l}\right) + (u-g)\ln\left(\frac{u-g}{u-1}\right)\right];$$

where $C = \frac{u-l}{(1-l)(u-1)}$.

These are the most commonly used functions in practice of calibration in official statistics, and appear most often in the standard calibration software packages.

## 3.2 A General Scheme for Deriving the Algorithms

This section presents a scheme for constructing a family of algorithms used in many of the calibration packages. This family of algorithms is derived using a similar approach to that outlined in [19], which uses a Newton-Raphson method to solve the calibration problem (6) .

### 3.2.1 The Function $h$

Let $h(x) = (\phi')^{-1}(x)$, i.e. $h$ is the inverse of $\phi'$. From the strong convexity of $\phi$, it can be deduced that $\phi'(g)$ is strictly increasing and so the inverse function $h$ is uniquely defined.

For the functions $\phi^{(Q)}$, $\phi^{(R)}$ and $\phi^{(L)}$ defined in Section 3.1, the corresponding $h$-functions are:

(i) Quadratic:
$$h^{(Q)}(x) = 1 + x;$$

(ii) Raking:
$$h^{(R)}(x) = \exp(x);$$

(iii) Logit:
$$h^{(L)}(x; l, u) = \frac{l(u-1) + u(1-l)\exp(Cx)}{(u-1) + (1-l)\exp(Cx)};$$

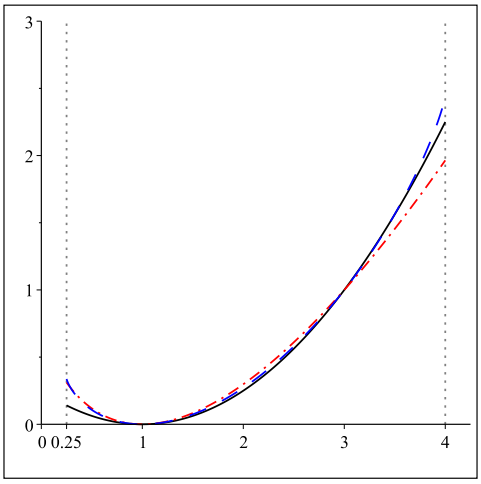
where $C$ is defined as in Section 3.1.

In Figure 1, each of the functions $\phi^{(Q)}$, $\phi^{(R)}$, and $\phi^{(L)}$ and their corresponding derivatives are plotted. Observe that for each of these functions their derivatives are strictly increasing.

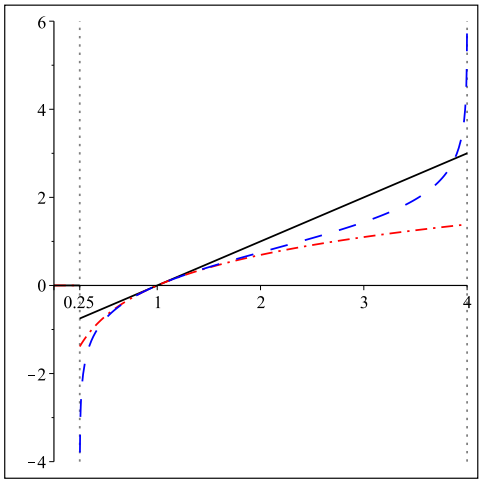
### 3.2.2 Lagrangian Method

Returning to the calibration problem (6), let $\Lambda = (\lambda_1 \ldots, \lambda_m)'$ be the $m$-vector of Lagrange multipliers. The Lagrangian for the problem (6) with function (7) can be written as:

$$\mathcal{L}(G, \Lambda) = \Phi(G) - \Lambda'(A'G - T) = \sum_{i=1}^{n} \phi(g_i) - \sum_{j=1}^{m} \lambda_j \left( \sum_{i=1}^{n} a_{ij} g_i - t_j \right).$$




(a) Functions $\phi^{(Q)}$ *(line)*, $\phi^{(R)}$ *(dash)*, and $\phi^{(L)}$ *(dot-dash)*




(b) Derivatives of the functions $\phi^{(Q)}$ *(line)*, $\phi^{(R)}$ *(dash)*, and $\phi^{(L)}$ *(dot-dash)*

Figure 1: Calibration penalty functions and their derivatives

Set $\phi'(g_i) = \frac{\partial\phi(g)}{\partial g}\Big|_{g=g_i}$. Differentiating $\mathcal{L}(G,\Lambda)$ with respect to $g_i$ $(i = 1,\ldots,n)$ gives

$$\frac{\partial\mathcal{L}(G,\Lambda)}{\partial g_i} = \phi'(g_i) - \sum_{j=1}^{m}\lambda_j a_{ij}.$$

Let $\mathbf{a}_i$ denote the $i$-th row of $A$, $i = 1,\ldots,n$ so that $\mathbf{a}_i = (a_{i1},\ldots,a_{im})$. Setting $\frac{\partial\mathcal{L}(G,\Lambda)}{\partial g_i} = 0$ gives

$$\phi'(g_i) = \sum_{j=1}^{m}\lambda_j a_{ij} = \mathbf{a}_i\Lambda. \tag{8}$$

Recall from Section 3.2.1 that $h(x) = (\phi')^{-1}(x)$. Then (8) implies that the $g$-weights $g_i$ $(i = 1,\ldots,n)$ corresponding to the vector $\Lambda$ of Lagrange multipliers is

$$g_i = h(\mathbf{a}_i\Lambda). \tag{9}$$

Applying the calibration constraint $A'G = T$, it follows from (9) it follows that

$$A'G = T \iff \sum_{i=1}^{n} \mathbf{a}_i' g_i = T \iff \sum_{i=1}^{n} \mathbf{a}_i' h(\mathbf{a}_i \Lambda) = T. \tag{10}$$

Note that Deville and Särndal in [19] proceed by subtracting $A'\mathbf{1} = \sum_{i=1}^{n} \mathbf{a}_i'$ from both sides of (10) and defining

$$\eta(\Lambda) = \sum_{i=1}^{n} \mathbf{a}_i' \left( h(\mathbf{a}_i \Lambda) - 1 \right);$$

however, this is not required here.

The objective is to solve the equation

$$\sum_{i=1}^{n} \mathbf{a}_i' h(\mathbf{a}_i \Lambda) = T, \tag{11}$$

with respect to $\Lambda$. Upon solving for $\Lambda$, the calibrated weights $G = (g_1, \ldots, g_n)'$ can be derived with $g_i = h(\mathbf{a}_i \Lambda)$ as given by (9).

Algorithms for solving (11) with respect to $\Lambda$ are now considered. This section considers the use of a Newton-Raphson method (described by Ypma in [64]) as presented by Deville and Särndal in [19]. The main algorithms considered have the form

$$\Lambda^{(s+1)} = \Lambda^{(s)} + (A'H^{(s)}A)^{-1}(T - A'G^{(s)}), \quad \text{for } s = 0, 1, 2, \ldots, \tag{12}$$

where $\Lambda^{(0)} = \mathbf{0}$, $G^{(s)}$ denotes the updated vector of $g$-weights at iteration $s$, and $H^{(s)}$ is an $n \times n$ diagonal matrix specified for each algorithm.

### 3.2.3 First Iteration

Setting $s = 0$, the first iteration in (12) can be written as

$$\Lambda^{(1)} = \Lambda^{(0)} + (A'H^{(0)}A)^{-1}(T - A'G^{(0)}).$$

For the algorithms outlined in the literature and implemented in the main statistical packages, $\Lambda^{(0)} = \mathbf{0}$, $H^{(0)} = I_n$ and $G^{(0)} = \mathbf{1}$. Thus the first iteration can be written as

$$\Lambda^{(1)} = (A'A)^{-1}(T - A'\mathbf{1}). \tag{13}$$

An important observation is that $\Lambda^{(1)}$ is independent of the choice of the function $\phi$. It is easy to see that (13) coincides with the vector $\Lambda$ that solves (11) in the case of function $h^{(Q)}$ with no constraints (that is, $l_i = -\infty$ and $u_i = \infty$ for all $i$). Also, it is well documented that the calibrated weights

$$W = (d_1 h^{(Q)}(\mathbf{a}_1\Lambda^{(1)}), \ldots, d_n h^{(Q)}(\mathbf{a}_n\Lambda^{(1)}))'$$

are equivalent to the weights obtained using generalized regression estimation (GREG), see [52].

### 3.2.4 Jacobian

Let $J(\Lambda)$ denote the Jacobian of $\sum_{i=1}^{n} \mathbf{a}_i' h(\mathbf{a}_i\Lambda)$ considered as a function of $\Lambda$. Then it follows that $J(\Lambda^{(s)}) = A'H^{(s)}A$, where

$$H^{(s)} = \mathrm{diag}(h'(\mathbf{a}_1\Lambda^{(s)}), \ldots, h'(\mathbf{a}_n\Lambda^{(s)}))$$

and

$$h'(\mathbf{a}_i\Lambda) = \left.\frac{\partial h(x)}{\partial x}\right|_{x=\mathbf{a}_i\Lambda}.$$

Applying the Newton-Raphson method to solve (11) for $\Lambda$ gives the iterative procedure:

$$\Lambda^{(s+1)} = \Lambda^{(s)} + (J(\Lambda^{(s)}))^{-1}(T - A'G^{(s)}). \tag{14}$$

This is a particular case of (12) with $H^{(s)}$ defined as above. This Newton-Raphson approach is proposed in [19]. In the next section, various choices of the matrix $H^{(s)}$ are considered.

### 3.2.5 The Matrix $H^{(s)}$

The following three forms of $H^{(s)}$ appear in the literature and existing software.

**Newton-Raphson:** In this case, the matrix $H^{(s)}$ is given by

$$H^{(s)} = \text{diag}(h'(\mathbf{a}_1\Lambda^{(s)}), \ldots, h'(\mathbf{a}_n\Lambda^{(s)})),$$

as described in Section 3.2.4. The method (14) requires computation of $J(\Lambda^{(s)}) = A'H^{(s)}A$ at each iteration. This Newton-Raphson approach is proposed in [19]. The method converges quickly in an ideal situation when computation is exact, but in practice this choice of $H^{(s)}$ can lead to an unstable algorithm.

**Identity Matrix:** For this case, the matrix $H^{(s)}$ is taken to be:

$$H^{(s)} = I_n$$

for all $s$, and so at each iteration the initial Jacobian $J(\Lambda^{(0)}) = A'A$ is used.

**Matrix with $g$-weights on the diagonal:** In this form, the matrix is given by

$$H^{(s)} = \text{diag}(h(\mathbf{a}_1\Lambda^{(s)}), \ldots, h(\mathbf{a}_n\Lambda^{(s)}));$$

the diagonal entries of $H^{(s)}$ are simply $G^{(s)}$, the values of the calibrated weights $G$ at the $s$-th iteration. Since these weights are computed at each iteration anyway, the matrix $H^{(s)}$ does not require additional computations, unlike the first method.

In Section 3.4, the convergence properties of the iterative procedure (12) shall be considered for these three forms of the matrix $H^{(s)}$.

### 3.2.6 $H^{(s)}$ for Various Calibration Functions

The forms of the matrix $H^{(s)}$ for the three calibration functions outlined in Section 3.1 shall be considered. The quadratic function $\phi^{(Q)}$ shall be considered in the case of no constraints and general constraints, the raking function $\phi^{(R)}$ in the case of non-negativity constraints and general constraints, and the logit function $\phi^{(L)}$ in the case of general constraints.

**Function $\phi^{(Q)}$ with No Constraints** In this case, the iterative method (12) converges in one iteration. The $g$-weights derived from this method correspond to the weights using the generalized regression estimator (see [52]). Note that, in this case, the Newton-Raphson and identity matrix are equivalent, since $h'^{(Q)}(x) = 1$ for all $x \in \mathbb{R}$. Since $h^{(Q)}(0) = 1$, the matrix with $g$-weights on the diagonal is equivalent to the identity matrix for the first iteration. Since only one iteration is performed for $\phi^{(Q)}$ with no constraints, this means that these two cases are also equivalent. Hence, for $\phi^{(Q)}$ with no constraints, all three cases of $H^{(s)}$ outlined in Section 3.2.5 are equivalent.

**Function $\phi^{(Q)}$ with General Constraints** In this case, the iterative method (12) may not converge in one iteration. A projection algorithm is used to ensure any $g$-weights $g_i$ $(i = 1, \ldots, n)$ that fall outside of the interval $[l_i, u_i]$ are projected back to this interval. Informally, if $g_i < l_i$, the weight is projected such that $g_i = l_i$; similarly, if $g_i > u_i$, it is projected such that $g_i = u_i$. The algorithm is then updated to account for this projection and the calibration is continued. See Section 3.3.4 for a full description of the algorithm. Note that in this case, the Newton-Raphson and identity matrix are equivalent, since $h'^{(Q)}(x) = 1$ for $x \in \mathbb{R}$. However, this method will now require more than one iteration, and so the matrix with $g$-weights on the diagonal will be different to the other matrices from the second iteration onwards.

**Function $\phi^{(R)}$ with Non-Negativity and General Constraints** The comments made in this section regarding $H^{(s)}$ for the function $\phi^{(R)}$ apply in both the cases of non-negativity constraints and general constraints. Observe that for

| Function | $g$-weight constraints | Newton-Raphson (I), Identity (II) and Matrix with $g$-weights (III) |
|---|---|---|
| $\phi^{(Q)}$ | $g \in (-\infty, \infty)$ | $(I) = (II) = (III)$ |
| $\phi^{(Q)}$ | $g \in [l_i, u_i]$ | $(I) = (II) \neq (III)$ |
| $\phi^{(R)}$ | $g \in [0, \infty)$ | $(I) = (III) \neq (II)$ |
| $\phi^{(R)}$ | $g \in [l_i, u_i]$ | $(I) = (III) \neq (II)$ |
| $\phi^{(L)}$ | $g \in [l_i, u_i]$ | $(I) \neq (II) \neq (III)$ |

Table 1: Comparisons of the three forms of the matrix $H^{(s)}$ for various calibration functions in different $g$-weight constraint cases

$x \in [0, \infty)$ the function $h^{(R)}$ and its derivative are identical, since $h^{(R)}$ is an exponential function, we deduce that $h'^{(R)}(x) = h^{(R)}(x) = \exp(x)$. Hence, the Newton-Raphson matrix and matrix with $g$-weights on the diagonal are equivalent. However, since $\exp(x) \neq 1$ for all $x \in [0, \infty)$, the identity matrix form of $H^{(s)}$ will be different to the other matrices from the second iteration onwards (note that, since $\exp(0) = 1$, all the matrices will be equal to the identity matrix at the first iteration). Due to the function definition, the non-negativity constraints are automatically taken into account with function $\phi^{(R)}$. However, for general constraints, a projection algorithm, similar to that for $\phi^{(Q)}$ with general constraints, is required (see Section 3.3.4).

**Function $\phi^{(L)}$ with General Constraints** Observe that for the function $\phi^{(L)}$, the inverse function $h^{(L)}(x)$ is such that $h'^{(L)}(x) \neq h^{(L)}(x)$ for all $x \in [l_i, u_i]$, hence the Newton-Raphson matrix and matrix with $g$-weights on the diagonal are not equivalent. Note also that $h'^{(L)}(x)$ and $h^{(L)}(x)$ are not equal to 1 for all $x \in [l_i, u_i]$, hence the identity matrix form of $H^{(s)}$ will be different to the other two forms from the second iteration onwards. Note that $h'^{(L)}(0) = h^{(L)}(0) = 1$, hence all three matrices will be equivalent for the first iteration.

Table 1 summarises this section. The functions, the $g$-weight constraints, and the relationships between the various forms of the matrix $H^{(s)}$ are given. Convergence properties of (12) shall be considered for all forms of the matrix $H^{(s)}$ in Section 3.4. However, before considering several examples, the algorithms for solving (11) using the iterative procedure (12) shall be described.

## 3.3 Algorithms

This section outlines several specific algorithms for solving the equation (11) using the iterative procedure (12).

### 3.3.1 The Main Algorithms

In this section, two of the main algorithms for solving the calibration problem (6) are described. Some alternative algorithms not presented in this chapter are briefly described in Section 3.5.

Any specific algorithm of the form (12) will be characterized by the following:

- Choice of the function $\phi$;
- Choice of the matrix $H^{(s)}$;
- Choice of the constraints on $G$ additional to the main calibration constraint $A'G = T$ (that is, choice of $L$ and $U$); and
- Choice of an appropriate stopping rule.

There are three main choices for the function $\phi$ as described in Section 3.1. There are also three choices for the matrix $H^{(s)}$; see Section 3.2.5. The three choices of the vectors $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$ were outlined in Section 3.1. The stopping rule used in all the algorithms described in this section is of the following type: STOP if either $A'G^{(s)} = T$ to within a pre-specified accuracy or the maximum number of iterations is met.

Two algorithms are considered that are used in many of the calibration software packages (see Chapter 3.6 for further details of these packages):

- Algorithm 1 is applicable to the function $\phi^{(L)}$ in the case of general constraints, and to function $\phi^{(R)}$ in the case of non-negativity constraints.
- Algorithm 2 is applicable to the functions $\phi^{(Q)}$ and $\phi^{(R)}$ in the case of general constraints.

### 3.3.2 Algorithm 1: No Projections Needed

**Input** Matrix $A$, vector $T$, vectors $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$, the form of the matrix $H^{(s)}$, and the function $\phi$ (either $\phi^{(L)}$ or $\phi^{(R)}$). For the function $\phi^{(R)}$, only the bounds $l_i = 0$ and $u_i = \infty$ for all $i = 1, \ldots n$ can be used. For the function $\phi^{(L)}$, $l_i \geq 0$ and $u_i < \infty$ for all $i = 1, \ldots n$.

**Output** The vector $G^{(s+1)}$ computed at the final iteration; this vector is the (approximate) solution of the calibration problem (6) for the chosen function $\phi$.

**Algorithm 1**

1. Set $s = 0, \Lambda^{(0)} = \mathbf{0}, G^{(0)} = \mathbf{1}$, and $H^{(0)} = I_n$.
2. Compute $\Lambda^{(s+1)} = (\lambda_1^{(s+1)}, \ldots, \lambda_m^{(s+1)})'$ using (12).
3. Compute $G^{(s+1)} = (g_1^{(s+1)}, \ldots, g_n^{(s+1)})'$ by $g_i^{(s+1)} = h(\mathbf{a}_i \Lambda^{(s+1)})$.
4. Compute $H^{(s+1)}$ as outlined in Section 3.2.4 using one of the three forms of $H^{(s)}$.
5. STOP if the stopping criterion is satisfied. Otherwise, set $s \to s + 1$ and return to 2.

Algorithm 1 is characterized by the following: an input matrix $A$, an input vector $T$, the form of the matrix $H^{(s)}$, the function $\phi^{(L)}$ or $\phi^{(R)}$, the vectors $L$ and $U$ in the case of function $\phi^{(L)}$, and the constraints for $g_i$ used. This algorithm cannot be used for $\phi^{(Q)}$ (unless no constraints are imposed on $g_i$, in which case the solution is obtained in the first iteration, see Section 3.3.3). For the function $\phi^{(R)}$, Algorithm 1 can only be used if the required constraint is the non-negativity constraint.

**Remark** Algorithm 1 cannot be used for $\phi^{(Q)}$ unless there are no constraints imposed on $g_i$; in this case, the solution is obtained in the first iteration, see Algorithm 1a below.

### 3.3.3 Algorithm 1a: Quadratic Function $\phi^{(Q)}$ with No Constraints

This method is non-iterative and contains the following two steps only:

1. Compute $\Lambda^{(1)}$ from (12) using $G^{(0)}$ and $H^{(0)}$.
2. Compute $G^{(1)} = \mathbf{1} + A'\Lambda^{(1)}$.

For the functions $\phi^{(Q)}$ and $\phi^{(R)}$ with general constraints, Algorithm 2 described below should be used.

### 3.3.4 Algorithm 2: Projections to the Additional Constraints Required

**Input** Matrix $A$, vector $T$, vectors $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$ such that $0 \leq l_i < 1 < u_i \leq \infty$ for all $i = 1, \ldots n$, form of the matrix $H^{(s)}$, and function $\phi$ (either $\phi^{(Q)}$ or $\phi^{(R)}$).

**Output** The vector $G^{(s+1)}$ computed at the final iteration; this vector is the (approximate) solution of the calibration problem (6) for the chosen function $\phi$.

**Algorithm 2**

1. Set $s = 0$, $n_0 = n$, $\Lambda^{(0)} = \mathbf{0}, G^{(0)} = \mathbf{1}$, $H^{(0)} = I_n$, $A^{(0)} = A$, $T^{(0)} = T$, $L^{(0)} = L$, and $U^{(0)} = U$.
2. Compute $\Lambda^{(s+1)} = (\lambda_1^{(s+1)}, \ldots, \lambda_m^{(s+1)})'$ by

$$\Lambda^{(s+1)} = \Lambda^{(s)} + ((A^{(s)})'H^{(s)}A^{(s)})^{-1}(T^{(s)} - (A^{(s)})'G^{(s)}), \tag{15}$$

   which is the formula (12) with $A = A^{(s)}$ and $T = T^{(s)}$.
3. Use Algorithm 2' below to compute $n_{s+1}$, matrix $A^{(s+1)}$ of size $n_{s+1} \times m$, vector $T^{(s+1)}$ of size $m$, and vectors $L^{(s+1)}$, $U^{(s+1)}$, and $G^{(s+1)}$ of size $n_{s+1}$.

4. Compute the matrix $H^{(s+1)}$ of size $n_{s+1} \times n_{s+1}$ as outlined in Section 3.2.4 with $A{=}A^{(s+1)}$ and $n = n_{s+1}$. For $s > 0$, the matrix $H^{(s)}$ is computed as outlined in Section 3.2.5 using one of the three forms of $H^{(s)}$. Here $\mathbf{a}_i^{(s)}$ denote $i$-th rows of $A^{(s)}$ so that $\mathbf{a}_i^{(s)} = (a_{i1}, \ldots, a_{im})$, $i = 1, \ldots, n_s$.

5. STOP if the stopping criterion is satisfied. Otherwise, set $s \to s + 1$ and return to Step 2.

### 3.3.5 Algorithm 2': Performing Step 3 in Algorithm 2

**Input** Matrix $A^{(s)} = (a_{ik}^{(s)})_{i,k}$ of size $n_s \times m$, vector $T^{(s)}$ of size $m$, the vectors $L^{(s)} = (l_1^{(s)}, \ldots, l_{n_s}^{(s)})'$ and $U^{(s)} = (u_1^{(s)}, \ldots, u_{n_s}^{(s)})'$ of size $n_s$.

**Output** Integer $n_{s+1} \leq n_s$, matrix $A^{(s+1)}$ of size $n_{s+1} \times m$, vector $T^{(s+1)}$ of size $m$, vectors $G^{(s+1)}$, $L^{(s+1)}$, and $U^{(s+1)}$ of size $n_{s+1}$.

**Algorithm 2'**

1. Compute the vector $\widetilde{G}^{(s+1)} = (\widetilde{g}_1^{(s+1)}, \ldots, \widetilde{g}_{n_s}^{(s+1)})'$ of size $n_s$, where $\widetilde{g}_i^{(s+1)} = h(\mathbf{a}_i^{(s)}\Lambda^{(s+1)})$, $i{=}1, \ldots, n_s$.

2. If $l_i^{(s)} \leq \widetilde{g}_i^{(s+1)} \leq u_i^{(s)}$ for all $i = 1, \ldots, n_s$ (i.e. all weights are within the required bounds), then set $n_{s+1} = n_s$, $A^{(s+1)} = A^{(s)}$, $G^{(s+1)} = \widetilde{G}^{(s+1)}$, $T^{(s+1)} = T^{(s)}$, $L^{(s+1)} = L^{(s)}$, and $U^{(s+1)} = U^{(s)}$. Otherwise go to the next step.

3. Define
$$\gamma_i^{(s+1)} = \begin{cases} \widetilde{g}_i^{(s+1)} & \text{if } l_i^{(s)} \leq \widetilde{g}_i^{(s+1)} \leq u_i^{(s)}; \\ l_i^{(s)} & \text{if } \widetilde{g}_i^{(s+1)} < l_i^{(s)}; \\ u_i^{(s)} & \text{if } \widetilde{g}_i^{(s+1)} > u_i^{(s)}. \end{cases} \tag{16}$$
The map (16) produces a split of the set of indices $\Omega^{(s)} = \{1, 2, \ldots, n_s\}$ into three subsets: $\Omega_l^{(s)}$, $\Omega_u^{(s)}$, and $\Omega_m^{(s)}$.

   Define $n_{s+1}$ to be the number of times the equality $\gamma_i^{(s+1)} = \widetilde{g}_i^{(s+1)}$ is satisfied. Let $\Omega_m^{(s)}{=}\{i_1, i_2, \ldots, i_{n_{s+1}}\}$ be the ordered set of indices such that the

equality $\gamma_i^{(s+1)} = \widetilde{g}_i^{(s+1)}$ holds for $i = i_j$, $j = 1, \ldots, n_{s+1}$. The indices in $\Omega_m^{(s)}$ are ordered so that $i_j < i_{j+1}$ for all $j$.

Similarly, $\Omega_l^{(s)}$ and $\Omega_u^{(s)}$ are defined as the ordered sets of indices such that the inequalities $\widetilde{g}_i^{(s+1)} < l_i^{(s)}$ or $\widetilde{g}_i^{(s+1)} > u_i^{(s)}$ hold, respectively, for the indices in $\Omega_l^{(s)}$ and $\Omega_u^{(s)}$.

4. Define the matrix $A^{(s+1)} = (a_{jk}^{(s+1)})_{j,k}$ of size $n_{s+1} \times m$ by $a_{jk}^{(s+1)} = a_{i_j k}^{(s)}$ for $j$=1, $\ldots$, $n_{s+1}$ such that $i_j \in \Omega_m^{(s)}$. Similarly, compute the vectors $G^{(s+1)}$=$(g_j^{(s+1)})_j$, $L^{(s+1)} = (l_j^{(s+1)})_j$, and $U^{(s+1)} = (u_j^{(s+1)})_j$ of size $n_{s+1}$ as follows: $g_j^{(s+1)} = \gamma_{i_j}^{(s+1)}$, $l_j^{(s+1)} = l_{i_j}^{(s)}$, and $u_j^{(s+1)}$=$u_{i_j}^{(s)}$, with the index $j = 1, \ldots, n_{s+1}$ such that $i_j \in \Omega_m^{(s)}$.

5. Let $\widetilde{n}_s = n_s - n_{s+1}$. Form $\Omega_l^{(s)} \cup \Omega_u^{(s)} = \{i_1, i_2, \ldots, i_{\widetilde{n}_s}\}$, the set of indices such that either of the inequalities $\widetilde{g}_i^{(s+1)} < l_i^{(s)}$ or $\widetilde{g}_i^{(s+1)} > u_i^{(s)}$ hold for $i = i_l$, $l$=1, $\ldots$, $\widetilde{n}_s$.

6. Define matrix $\tilde{A}^{(s+1)} = (a_{lk}^{(s+1)})_{l,k}$ of size $\widetilde{n}_s \times m$ by $a_{lk}^{(s+1)} = a_{i_l k}^{(s)}$ for $l = 1, \ldots, \widetilde{n}_s$ such that $i_l \in \Omega_l^{(s)} \cup \Omega_u^{(s)}$. Similarly, compute vector $\tilde{G}^{(s+1)} = (g_l^{(s+1)})_l$ of size $\widetilde{n}_s$ as $g_l^{(s+1)} = \gamma_{i_l}^{(s+1)}$ for $l = 1, \ldots, \widetilde{n}_s$ such that $i_l \in \Omega_l^{(s)} \cup \Omega_u^{(s)}$.

7. Compute $T^{(s+1)} = T^{(s)} - (\tilde{A}^{(s+1)})' \tilde{G}^{(s+1)}$.

## 3.4 Examples

In this section, various examples are considered to explore the convergence properties of the algorithms described in Section 3.3. To begin, Algorithm 1 is considered for function $\phi^{(L)}$ with general constraints. It is show that, for this case, there are three types of convergence. In the second example, properties of the calibrated weights at subsequent iterations of Algorithms 1 and 2 are explored. The section concludes by considering convergence properties of both Algorithms 1 and 2 for all possible combination of functions with various choices of the matrix $H^{(s)}$.

**Example 1: Convergence Properties of Algorithm 1 for $\phi^{(L)}$ with General Constraints**

In this example, the behaviour of Algorithm 1 for the function $\phi^{(L)}$ is explored. There are three interesting cases to consider:

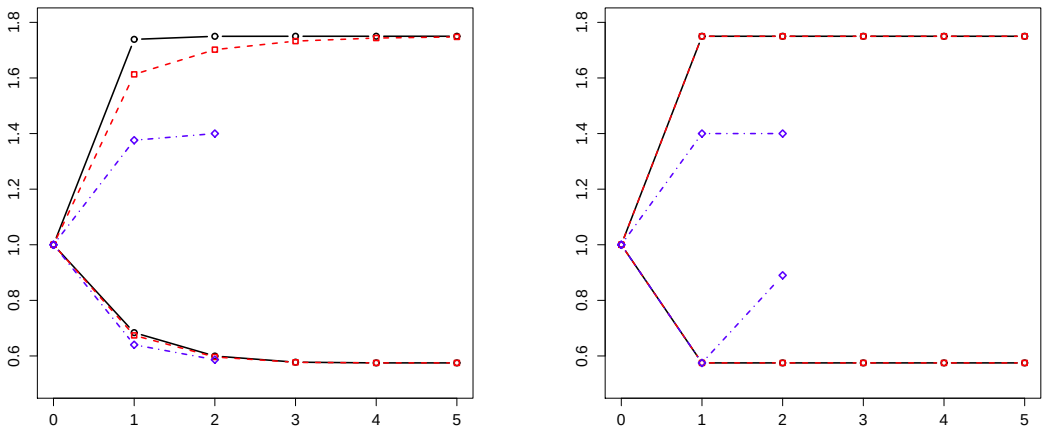
1. If the constraint $A'G = T$ cannot be satisfied, then the algorithm does not converge and gives bad or no results.
2. If the constraint $A'G = T$ can be satisfied but some of the weights $g_i$ tend to $l_i$ or $u_i$, then the algorithm gives slow or no convergence.
3. If $A'G = T$ can be satisfied and all the weights $g_i$ remain well within the bounds imposed by $l_i$ and $u_i$, then the algorithm converges quickly.

Each of these cases shall be illustrated using a small toy example. Take the vector $T = (6.4, 12.2)'$ and $l_1 = l_2 = l = 0.5$. Algorithm 1 is used with the function $\phi^{(L)}$ and general constraints. Only the Newton-Raphson form of the matrix $H^{(s)}$ shall be considered in this example. Set $A = (\mathbf{a}_1, \mathbf{a}_2)'$ where $\mathbf{a}_1 = (2, 6)$ and $\mathbf{a}_2 = (3, 5)$. The value of $u_1 = u_2 = u$ shall be varied to illustrate each of the three cases described above.

For comparison purposes, the convergence properties of Algorithm 2 for the function $\phi^{(Q)}$ in the case of general constraints shall also be considered. However, for Algorithm 2 using $\phi^{(Q)}$ there are only two cases - convergence or no convergence.

**Case 1 - Fast Convergence** Begin by taking $u = 2$. After five iterations of Algorithm 1, the vector $A'G - T$ has both elements of order $10^{-8}$, thus after five iterations the constraints have essentially been satisfied. The algorithm continues to improve in accuracy, and after 11 iterations of Algorithm 1, $A'G - T$ has infinitesimally small elements. The determinant of the final Jacobian matrix is approximately 8.55. Since the $g$-weights do not approach $l$ or $u$, there are no issues with infinite values appearing in the Jacobian matrix (recall that the derivative of $\phi^{(L)}$ is infinite at $l$ and $u$). For this case, the weights converge to $G = (0.575, 1.75)'$ very quickly. The weights for each iteration of Algorithm 1 are plotted in Fig-

ure 2(a) (circle, line, black). Contrast this to the weights in Figure 2(b), where Algorithm 2 for $\phi^{(Q)}$ has converged after one iteration.




(a) $g$-weights using Algorithm 1 for $\phi^{(L)}$

(b) $g$-weights using Algorithm 2 for $\phi^{(Q)}$

Figure 2: Plot of $g$-weights for the first 5 iterations of Algorithm 1 for $\phi^{(L)}$ and Algorithm 2 for $\phi^{(Q)}$ in different cases of convergence; convergence when $u = 2$ *(black, circle, line)*, convergence when $u = 1.75$ *(red, square, dash)* and convergence when $u = 1.4$ *(blue, diamond, dot-dash)*

**Case 2 - Slow Convergence** Now consider the value of $u$ as 1.75, the value to which the larger weight converged in Case 1. Re-running Algorithm 1 in this case gives much slower convergence. After 5 iterations of Algorithm 1, the vector $A'G - T$ has elements -0.007 and -0.012. The determinant of the Jacobian matrix is 0.319, which is much smaller than the corresponding value in Case 1. After 12 iterations of Algorithm 1, $G = (0.575, 1.749)'$. The elements of $A'G - T$ are of order $10^{-5}$, larger than the values of $A'G - T$ after five iterations in Case 1. The determinant of the Jacobian matrix after 12 iterations is 2.91 $\times 10^{-4}$. This continues to decrease with subsequent iterations, reaching an infinitesimally small value after 50 iterations. The algorithm continues to move slowly towards the solution $G = (0.575, 1.75)'$; however, the algorithm fails to reach the upper bound of 1.75, since reaching this upper bound would lead to an infinite value in the Jacobian matrix (recall that the derivative of $\phi^{(L)}$ is $\infty$ at $u$). The weights for the first five iterations of Algorithm 1 are plotted in Figure 2(a) (square, dash,

| Case | $u$ | No. of iter | $A'G - T$ |
|---|---|---|---|
| Fast convergence | 2 | 5 | $10^{-8}$ |
| Slow convergence | 1.75 | 11 | $10^{-5}$ |
| No convergence | 1.4 | 3 (then stop) | 1 |

Table 2: Convergence properties of Algorithm 1 for $\phi^{(L)}$ in Example 1 for various values of $u$ with $l = 0.575$

red). Contrast this with the weights for Algorithm 2 with function $\phi^{(Q)}$, plotted in Figure 2(b), where once again the algorithm converges in one iteration.

**Case 3 - No Convergence** Finally, the value of $u$ is taken to be 1.4. In this case, the algorithm runs for three iterations. At the third iteration, the value of the weights are $G = (0.576, 1.400)'$; however, the entries of $A'G - T$ are -1.049 and -1.746. Therefore, the calibration constraints are not satisfied. The determinant of the Jacobian matrix after three iterations is $2.75 \times 10^{-7}$. This small value of the determinant, together with the upper weight virtually reaching the upper bound of 1.4, causes the algorithm to fail when trying to invert the Jacobian matrix. The matrix will have an infinitely large entry as well as an infinitesimally small determinant, both of which cause the algorithm to fail. The trajectory of the weights in this case is plotted in Figure 2(a) (diamond, dot-dash, blue). Figure 2(b) shows the trajectory of the weights for Algorithm 2 with function $\phi^{(Q)}$, which also runs for three iterations but fails to converge. Observe that the weights at the third iteration for Algorithm 2 with function $\phi^{(Q)}$ are different to those for the third iteration of Algorithm 1 with function $\phi^{(L)}$. The algorithms are behaving differently in an attempt to find a solution to the calibration problem which, in this case, does not have a solution.

Table 2 summarizes the key points from this example. To conclude this example, some brief remarks are given regarding Algorithms 1 and 2.

**Multi-start** Algorithms 1 and 2 were started for various $\Lambda^{(0)}$ in both Cases 1 and 2 above. For suitable choices of $\Lambda^{(0)}$ (in particular, such that $h(\mathbf{a}_i\Lambda^{(0)})$ gave weights $g_i$ in the range $l_i \leq g_i \leq u_i$, $i = 1, \ldots, n$), the algorithms converged to the

same solution. The final $g$-weights $g_i$ $(i = 1, \ldots, n)$ and the Lagrange multipliers $\Lambda$ were the same in all cases (to within computer accuracy).

**Derivatives** The identities $\phi'(g_i) = \mathbf{a}_i\Lambda$ and $g_i = h(\mathbf{a}_i\Lambda)$ were confirmed for the final value of the Lagrange multipliers $\Lambda$ and the calibrated weights $g_i$ given by Algorithms 1 and 2. This suggests that the algorithms have converged to a (local) minimum.

**Example 2: Investigation of Calibrated Weights at Each Iteration of Algorithms 1 and 2**

In this example, the convergence properties of Algorithms 1 and 2 are further explored by considering the calibrated weights at each iteration of the algorithms.

**Data** In this example, the Belgian municipalities dataset included in the 'sampling' package in R is considered (see [61] for more details). The dataset provides information about the Belgian population on July 1st 2004 compared with July 1st 2003, and includes financial information about the municipality incomes at the end of 2001. Data is available for the 589 municipalities in Belgium. There are 17 variables in the dataset, including the municipality name and province number. However, the 8 variables of interest in this example are the number of men on July 1st 2003, the number of women on July 1st 2003, the difference in the number of men on July 1st 2003 and July 1st 2004, the difference in the number of women on July 1st 2003 and July 1st 2004, total taxable income in Euros in 2001, total taxation in Euros in 2001, average of the income-tax return in Euros in 2001 and the median of the income-tax return in Euros in 2001.

A simple random sample of size 200 is taken and initial weights $d_i$=$N/n$ assigned where $N$ is the size of the population and $n$ is the sample size (in this example $N = 589$ and $n = 200$). These would be the weights used in the Horvitz-Thompson estimator [28]. The values of the 8 variables of interest for each of the 200 sample members are used to form the $200 \times 8$ matrix $X$. The matrix $A$ is formed using the relationship $a_{ij} = d_i x_{ij}$. Using Algorithm 1, this sample is calibrated to the

known totals for each of the 8 variables. These known totals are used to form the $8 \times 1$ vector $T$. Take $l_i = l = 0.73$ and $u_i = u = 1.3$ for $i = 1, \ldots, 200$.

**Calibrated Weights** For this section, we use the following abbreviations:

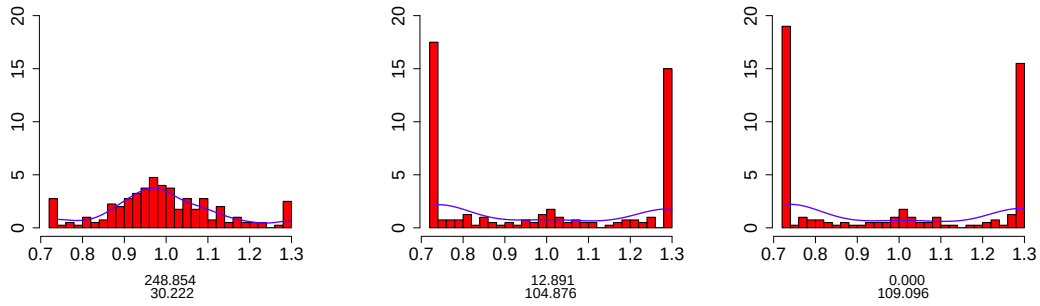
- **Method 1:** Refers to the use of Algorithm 2 (and 2') for the quadratic function $\phi^{(Q)}$ with general constraints.
- **Method 2:** Refers to the use of Algorithm 1 using the logit function $\phi^{(L)}$ with general constraints.

Figures 3 and 4 show histograms and the corresponding density plots of the weights at iteration 1 (see Figures 3(a) and 4(a)), iteration 5 (see Figure 3(b) and 4(b)), and the final iteration (see Figure 3(c) and 4(c)) using methods 1 and 2, respectively. The values of $||A'G - T||_F$ and $\phi^{(Q)}$ at that iteration are included below the plots.

After the first iteration, most of the $g$-weights stay close to their initial value of 1. Figure 3(a) shows a uni-modal distribution of the $g$-weights after the first iteration with the mode approximately 1. However, for the there are small peaks at both ends of the histogram. This is due to some of the calibrated weights being projected to the bounds by Algorithm 2'. By contrast, the are fewer weights at the bounds in Figure 4(a), since this method automatically takes the bounds into account.

For both methods, as the number of iterations increases, more weights are projected to the bounds of $l = l_i = 0.73$ or $u = u_i = 1.3$ (for $i = 1, \ldots, n$), leading to a bi-modal distribution with modes at $l$ and $u$. After the first iteration, there are approximately 5% of the weights at each bound; however, there are over 30% of the weights at each bound by the final iteration. As the number of iterations increases, there are fewer weights between $l$ and $u$. Observe that the value of $||A'G - T||_F$ decreases over subsequent iterations whilst the value of $\phi^{(Q)}/\phi^{(L)}$ increases.

In Figure 5(a), the weights using methods 1 and 2 are plotted and ordered by size. The red curve in Figure 5(a) corresponds to the weights (ordered by size) obtained

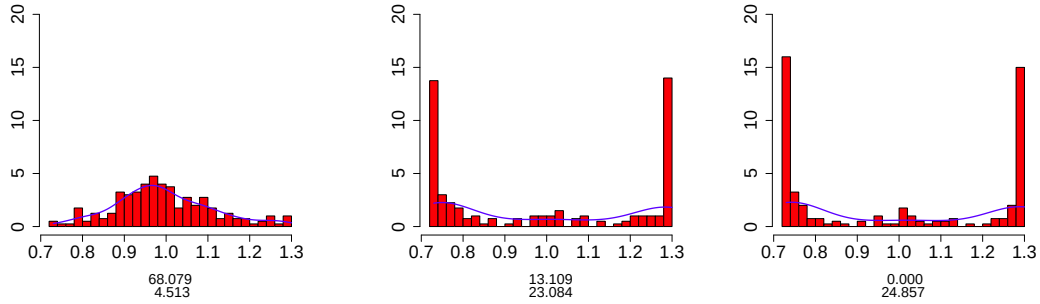



(a) $g$-weights at the 1st iteration

(b) $g$-weights at the 5th iteration

(c) $g$-weights at the final (8th) iteration

Figure 3: Histogram *(red)* and density plot *(blue line)* of $g$-weights for the quadratic function $\phi^{(Q)}$ at iterations 1, 5, and 8 with the values of $||A'G - T||_F$ and $\phi^{(Q)}$ at that iteration




(a) $g$-weights at the 1st iteration

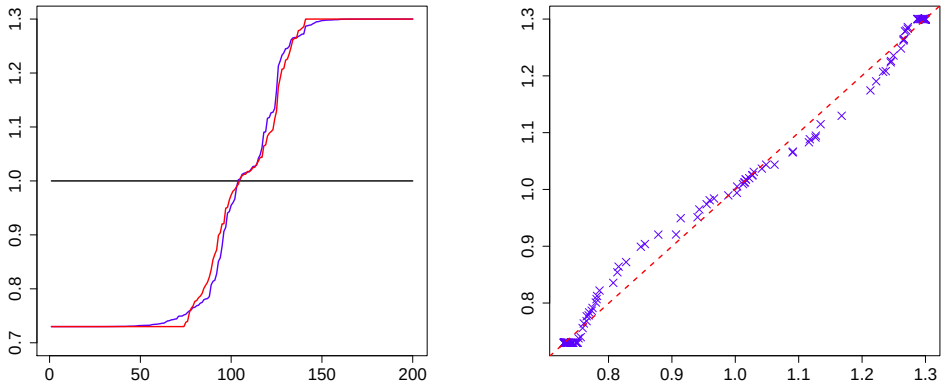
(b) $g$-weights at the 5th iteration

(c) $g$-weights at the final (9th) iteration

Figure 4: Histogram *(red)* and density plot *(blue line)* of $g$-weights for the logit function $\phi^{(L)}$ at iterations 1, 5, and 9 with the values of $||A'G - T||_F$ and $\phi^{(L)}$ at that iteration

using method 1, whilst the blue curve corresponds to the weights (ordered by size) obtained using method 2. Observe the red horizontal lines at $l = 0.73$ and $u = 1.3$. These show the weights that have been projected to the bounds. In contrast, the blue curve in has these horizontal lines as asymptotes (recall that method 2 cannot give weights at the bounds).

Figure 5(b) shows a scatter-plot of the calibrated weights for method 1 against the calibrated weights for method 2. These correspond to the weights given in Figures 3(c) and 4(c), respectively. Observe that there is a cluster of points that are horizontal in the upper right and lower left of the plot. This shows the weights




(a) Plot of $g$-weights for $\phi^{(Q)}$ *(red)* and $\phi^{(L)}$ *(blue)* against 1 *(black)*

(b) Scatter-plot of $g$-weights for $\phi^{(Q)}$ against $g$-weights for $\phi^{(L)}$

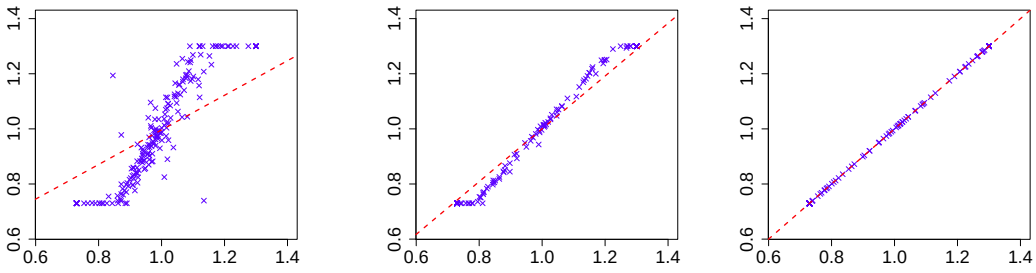
Figure 5: Investigating $g$-weights for the quadratic and logit functions in the case of general constraints

that were projected to the bounds for the quadratic function $\phi^{(Q)}$, but were not able to reach these bounds when the logit function $\phi^{(L)}$ was used.

To further investigate how the algorithms perform, the behaviour of the calibrated weights between subsequent iterations of the algorithms shall be investigated. Note that the scatter-plots of $g$-weights from the first iteration against the initial $g$-weights would give a vertical line of points at 1 on the horizontal axis. This is due to the fact that $G^{(0)} = \mathbf{1}$.

Figures 6 and 7 show scatter plots of the weights methods 1 and 2 at the $i$th iteration against the weights obtained at the $(i-1)$th iteration for $i = 2$, $i = 6$ and $i = 8/i = 9$ (method 1/2 respectively) (note that 0th iteration here refers to the initial weights). Observe the horizontal lines in Figures 6(a) and 6(b). These correspond to weights that were projected to the boundary values of $l$ and $u$ at the $i$-th iteration, which were not at the bounds at the $(i-1)$-th iteration. There are many of these weights in Figure 6(a), with fewer in Figure 6(b), and none in Figure 6(c). During the final iteration, there are few changes in the weights, as the algorithm has almost converged to the true solution.

Unlike the scatter-plots in Figure 6, the scatter-plots in Figure 7 do not have horizontal lines of weights. Instead, the arrangement of points resembles an

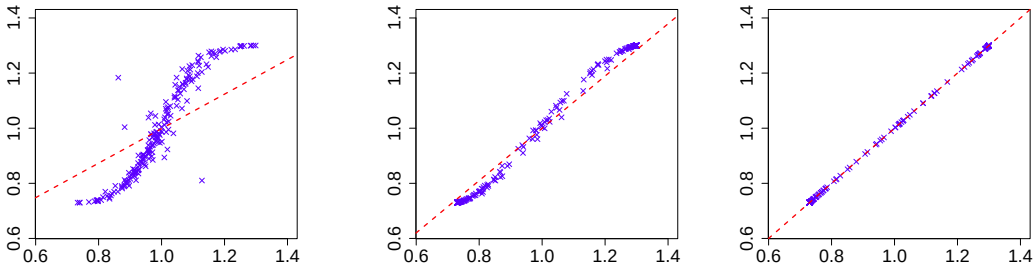



(a) $g$-weights at the 2nd iteration against the 1st iteration

(b) $g$-weights at the 6th iteration against the 5th iteration

(c) $g$-weights at the 8th iteration against the 7th iteration

Figure 6: Scatter-plot of weights for the quadratic function $\phi^{(Q)}$ at the $i$th iteration compared with the $(i-1)$-th iteration $(i = 2, 6, 8)$




(a) $g$-weights at the 2nd iteration against the 1st iteration

(b) $g$-weights at the 6th iteration against the 5th iteration

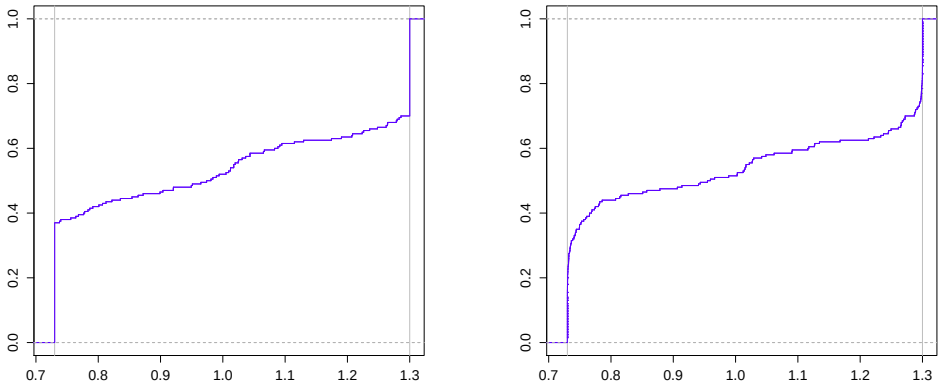
(c) $g$-weights at the 9th iteration against the 8th iteration

Figure 7: Scatter-plot of weights for the logit function $\phi^{(L)}$ at the $i$th iteration compared with the $(i-1)$-th iteration $(i = 2, 6, 9)$

'elongated-S' (see Figures 7(a) and 7(b)). This curvature of the points shows the weights that have moved nearer the bounds than in the previous iteration. However, these weights have not reached the boundary due to the infinite derivatives of the function $\phi^{(L)}$ at $l$ and $u$. There is little change in the calibrated weights as the algorithm nears convergence as shown in Figure 6(c) where almost all of the points lie on the main diagonal.

Figures 8(a) and 8(b) show the empirical cumulative distribution function for the weights in Figures 3(c) and 4(c) respectively; these are the weights at the final iteration using methods 1 and 2 respectively. Note that in Figure 3(c) the distribution is discontinuous at the lower and upper bounds of $l = 0.73$ and

$u = 1.3$, respectively. This is because many of the weights using Method 1 have been projected to the bounds. In Figure 4(c), there is a continuous distribution from $l$ to $u$, with the distribution curve becoming steeper near the bounds of $l$ and $u$. This plot further shows that, in the case of the logit function, the weights are tending to but cannot reach the bounds (due to the infinite value of the derivative of the function at the bounds).




(a) ECDF of the $g$-weights for $\phi^{(Q)}$ using Algorithm 2

(b) ECDF of the $g$-weights for $\phi^{(L)}$ using Algorithm 1

Figure 8: Empirical cumulative distribution function (ECDF) of the $g$-weights for functions $\phi^{(Q)}$ and $\phi^{(L)}$

**Comparison of Calibrated Weights when Projected to the Lower and Upper Bounds** The calibrated weights obtained using the logit function $\phi^{(L)}$ often tend towards, but cannot reach, the lower and upper bounds. This is in contrast to the weights obtained using Algorithm 2 for $\phi^{(Q)}$ with general constraints where the algorithm may lead to $g$-weights that do not satisfy the constraints $L \leq G \leq U$. In this case, Algorithm 2' is used to project any weights back to the nearest bound, before adjusting the remaining weights to satisfy the constraint $A'G = T$.

Now consider a similar procedure for the logit function $\phi^{(L)}$. In this case, the effect of projecting some of the calibrated weights to the lower bound $l$ and the upper bound $u$ shall be explored. The dataset is then re-calibrated using only the weights that have not been projected. This is continued until the constraint

$A'G = T$ is satisfied (as in Algorithm 2'). In Table 3, the function value $\phi^{(L)}$, the Frobenius norm of the distance from constraints $||A'G - T||_F$, and the coefficient of variation (CoV) of calibrated weights in various cases of projection are given. Note that the coefficient of variation (CoV) of the calibrated weights is related to variance of the corresponding calibration estimators. This is described by Kish in [31].

| Projection | $\phi^{(L)}(G)$ | $\|\|A'G - T\|\|_F$ | CoV |
|---|---|---|---|
| No projection | 91.74 | $3.04 \times 10^{-19}$ | 50.74 |
| The 45 largest and 45 smallest weights | 92.43 | $1.04 \times 10^{-17}$ | 50.50 |
| Weights within 0.05 of $l$ and $u$ | 92.94 | $4.73 \times 10^{-19}$ | 50.38 |
| The lower and upper 25% of the weights | 92.69 | $9.75 \times 10^{-17}$ | 50.67 |
| Weights below $l/0.975$ and above $0.975u$ | 92.04 | $6.11 \times 10^{-12}$ | 50.62 |

Table 3: Values of objective function $\phi^{(L)}$, Frobenius distance from constraints $||A'G - T||_F$ and coefficient of variation (CoV) for various cases of projections of weights to the lower and upper bounds

From Table 3, observe that the value of the objective function $\phi^{(L)}$ has increased in all cases of projections. Since the function $\phi^{(L)}$ has infinite derivative at $l$ and $u$, the function increases sharply near the bounds. Hence, any projection of weights is likely to increase the value of the objective function. However, the coefficient of variation of the weights is smaller when projections are used than in the case of no projection. As the projection moves the projected weights to the bounds, the remaining weights that are re-calibrated move nearer to 1 to account for this adjustment. This leads to a reduced variance and hence reduced coefficient of variation of the weights.

**Estimating the Total Number of People** Whilst the $g$-weights play an important role in the calibration problem, the main use of these weights is to estimate some quantity of interest. The properties of this estimator are often more interesting to practitioners than the properties of the weights themselves. The calibrated weights shall be used to estimate the number of people living in Belgium in 2004. This is done by taking 10,000 random samples from the Belgian municipalities dataset. Three methods shall be considered:

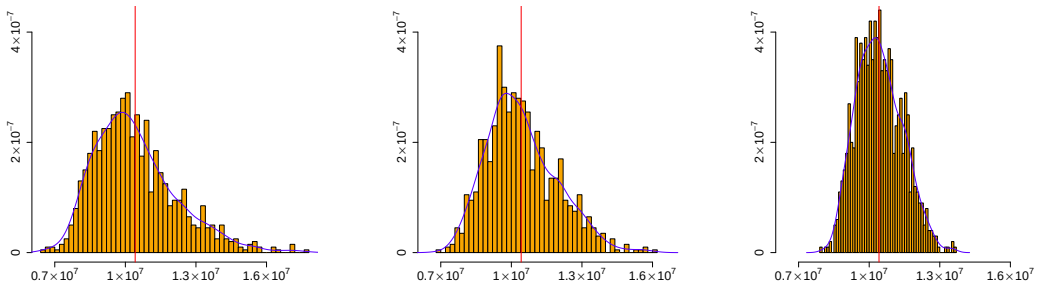
- *Method 1:* The Horvitz-Thompson estimator $Y'D$;
- *Method 2:* The calibration estimator $Y'W$ for the calibrated weights $W$ using Algorithm 2 with the quadratic function $\phi^{(Q)}$ in the case of general constraints; and
- *Method 3:* The calibration estimator $Y'W$ for the calibrated weights $W$ using Algorithm 1 with the logit function $\phi^{(L)}$ in the case of general constraints.

For each estimator, properties of the estimates when taking simple random samples of size 75, 100, and 200 shall be considered.

Figures 9, 10 and 11 show the distribution of the estimates for the true value of 10417122 when using methods 1, 2 and 3 described above, respectively. Sample sizes $n = 75$, $n = 100$ and $n = 200$ are considered for each method. As expected, the distribution of the estimators has a smaller variance as the sample size is increased.

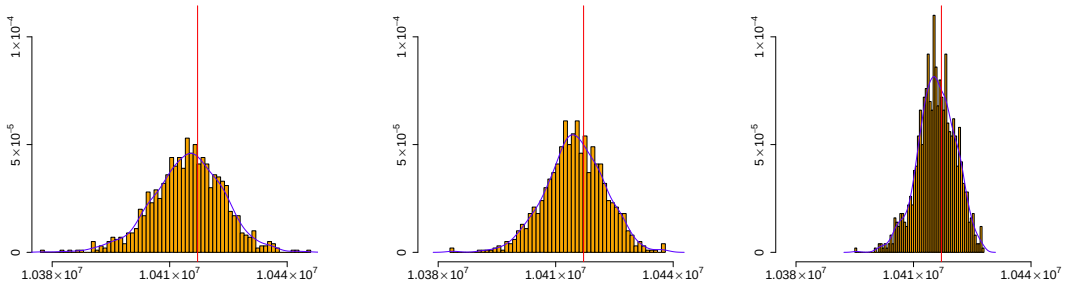
The distribution of estimates using the Horvitz-Thompson estimator is skewed to the left, with the mode of the distribution to the left of the true value. This skewness reduces as the sample size increases. The range of the estimates for the second and third methods is approximately 170 times smaller than the range of the estimates using the Horvitz-Thompson estimator. The distribution of the estimates in this case is less skewed than for the Horvitz-Thompson estimator, with the mode of the estimates close to the true value in all cases. This illustrates a key finding that, in general, calibration estimators give more reliable estimates in both the sense of being less variable and less skewed.

From the estimates in Figures 9, 10 and 11, the mean, bias, median, variance, and MSE of the estimates are computed. These values are given in Tables 4, 5 and 6 respectively. Surprisingly for the HT estimates, the bias is smallest when using the smallest sample size. However, the variance and MSE of the estimates in all cases decrease as the sample size increases, as expected. The variances, biases and MSE are smaller for the calibration estimators compared with the HT estimator. This illustrates the use of calibration as a method for reducing the sample variance of estimates.



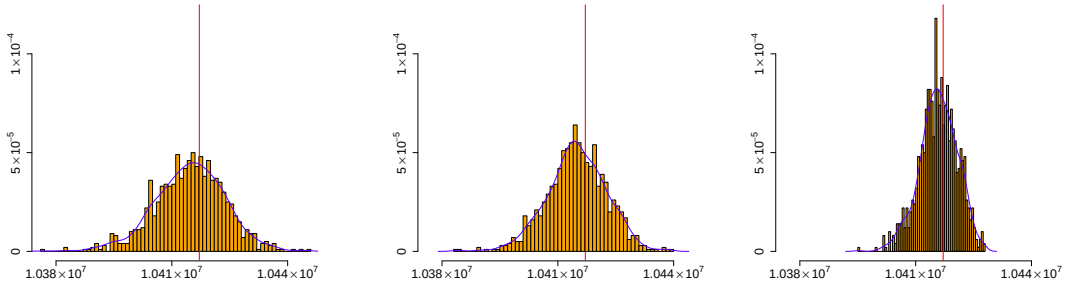

(a) Sample size $n = 75$ (b) Sample size $n = 100$ (c) Sample size $n = 200$

Figure 9: Estimates of the Belgian population in 2004 from 10,000 random samples of size 75, 100, and 200 using the Horvitz-Thompson estimator




(a) Sample size $n = 75$ (b) Sample size $n = 100$ (c) Sample size $n = 200$

Figure 10: Estimates of the Belgian population in 2004 from 10,000 random samples of size 75, 100, and 200 using the quadratic function $\phi^{(Q)}$




(a) Sample size $n = 75$ (b) Sample size $n = 100$ (c) Sample size $n = 200$

Figure 11: Estimates of the Belgian population in 2004 from 10,000 random samples of size 75, 100, and 200 using the logit function $\phi^{(L)}$

Furthermore, the median of the weights moves closer to the true value as the sample size increases in all cases. However, for methods 2 and 3 the values of the median are closer to the true value than for the corresponding estimates obtained using the HT estimator. This illustrates how calibration can lead to more reliable estimates.

Note that the values for the mean, bias, median, variance, and MSE are very similar to the values obtained using the estimates for the quadratic function $\phi^{(Q)}$. This agrees with the assertion in [19] that, under certain regularity conditions, the calibration estimators are asymptotically equivalent independent of the chosen penalty function.

| Horvitz-Thompson | $n = 75$ | $n = 100$ | $n = 200$ |
|---|---|---|---|
| Mean | 10425081 | 10439499 | 10437165 |
| Bias | 7959 | 22377 | 20043 |
| Median | 10146880 | 10236770 | 10355954 |
| Variance | $3.10475 \times 10^{12}$ | $2.21299 \times 10^{12}$ | $9.38258 \times 10^{11}$ |
| MSE | $3.10481 \times 10^{12}$ | $2.21349 \times 10^{12}$ | $9.38660 \times 10^{11}$ |

Table 4: Summary of estimates for the Belgian population in 2004 from 10,000 random samples of size 75, 100, and 200 using the Horvitz-Thompson estimator

| $\phi^{(Q)}$ | $n = 75$ | $n = 100$ | $n = 200$ |
|---|---|---|---|
| Mean | 10414658 | 10414928 | 10415853 |
| Bias | -2464 | -2194 | -1269 |
| Median | 10414893 | 10415008 | 10415837 |
| Variance | $8.14258 \times 10^7$ | $5.83535 \times 10^7$ | $2.38957 \times 10^7$ |
| MSE | $8.74984 \times 10^7$ | $6.31651 \times 10^7$ | $2.55059 \times 10^7$ |

Table 5: Summary of estimates for the Belgian population in 2004 from 10,000 random samples of size 75, 100, and 200 using the quadratic function $\phi^{(Q)}$

| $\phi^{(L)}$ | $n = 75$ | $n = 100$ | $n = 200$ |
|---|---|---|---|
| Mean | 10414669 | 10414918 | 10415888 |
| Bias | -2453 | -2204 | -1234 |
| Median | 10415042 | 10414850 | 10415894 |
| Variance | $8.27775 \times 10^7$ | $5.93664 \times 10^7$ | $2.40143 \times 10^7$ |
| MSE | $8.87961 \times 10^7$ | $6.42240 \times 10^7$ | $2.55367 \times 10^7$ |

Table 6: Summary of estimates for the Belgian population in 2004 using 10,000 random samples of size 75, 100, and 200 for the logit function $\phi^{(L)}$

These results have highlighted that the Horvitz-Thompson estimator gives estimates with larger variance than the estimates obtained from calibration. This

supports the motivation for calibration described in Section 1.2 that the use of calibration can lead to a reduction in the sampling variance of the estimates. In this example, the range of the Horvitz-Thompson estimates was approximately 170 times larger than the range of the calibrated estimates. The calibrated estimates generally perform better for estimating the true value than the estimates using the Horvitz-Thompson estimator (despite the Horvitz-Thompson estimator being unbiased, see [28]). However, in this example, the choice of the penalty function had little effect on the properties of the resulting estimates.

### Example 3: Convergence Properties of Algorithms 1 and 2 for Various Choices of $H^{(s)}$

The Labour Force Survey (LFS) is arguably one of the most important social surveys conducted by the Office for National Statistics (ONS). It is a household survey, where participants are asked about labour force characteristics and related topics. One labour force characteristic of interest is employment status, since this key information is used to calculate estimates of the UK employment and unemployment rate, statistics that are of interest to government, businesses, and even the general public.

Since 1992, the LFS has been carried out quarterly. Each selected household remains part of the sample for five consecutive quarters. This means one fifth of the sample needs to be replaced every quarter. The original purpose of the survey was to investigate characteristics for cross-sectional data. However, since households are retained in the survey for five consecutive quarters, it was recognised that the LFS could also be used to investigate characteristic changes of individuals across quarters. Sample members who respond in all five consecutive quarters can be linked and combined to give the so-called five-quarterly longitudinal LFS datasets.

The quarterly LFS began, in its current form, during the Spring of 1992. However, the rotating panel design of the sample (i.e., retaining households for five consecutive quarters and updating a fifth of the sample each quarter) was not established until Spring 1993, with the first five-quarterly LFS dataset considering households over the five-quarter period from Spring 1993 to Spring 1994. Every

quarter, a new five-quarterly LFS dataset is produced as another cross-sectional dataset becomes available.

However, combining five consecutive quarters' worth of cross-sectional datasets, and including only those sample members who responded in all five quarters, can lead to methodological issues and result in a sample that is unrepresentative of the true population. These issues can be classified by two main problems: firstly, this linking of the five datasets can result in bias due to non-response and attrition of the sample; secondly, there is the issue of bias that can occur due to response errors, since these can have a major effect on the estimates of changes in the characteristics of interest. See [58] for details of existing methodologies to deal with these issues.

The primary purpose of the longitudinal datasets is to produce estimates of flows, i.e. changes in characteristics over the five-quarterly period. In particular, the labour force flows are of particular interest, since these show patterns of people moving between states of employment, unemployment, and inactive as well as highlighting changes in the numbers of those who are of working age. For the five-quarterly LFS datasets, the flow characteristics can be considered as measuring the change in characteristics over a 12-month period.

As the dataset in consideration is used for forming estimates related to the working age population, that is, all males and females who are aged 16-69, only sample members who responded to all five waves of the LFS who were aged between 15 and 69 at wave 1 are included.

In this example, the five-quarterly longitudinal dataset for the five quarters from April 2012 to June 2013 is considered (see [42]). The working age population is estimated to be 44,443,746 from census data. There are 4538 sample members in the dataset. For each of these sample members, calibration is performed on 61 constraints. These constraints include satisfying known population totals in 28 age-sex categories, 18 region groups, and ensuring that the estimate of numbers of people in the three employment statuses (employed, unemployed, and inactive) matches each of the totals for each of the five quarters used to form the dataset.

Therefore, for this dataset, the values of $n$ (sample size) and $m$ (number of constraints) are $n = 4538$ and $m = 61$. The main purpose of the calibration here is consistency between the estimates of the population totals for each of the 61 constraints and their known totals. However, calibration can also help to deal with biases arising from non-response and sample design (see, for example, [37]).

Forming estimates of changes in employment status forms an important part of government policy, since the statistics produced highlight how employment has changed over the 12-month period. The estimates also show the numbers of those moving into and out of working age, which forms a key basis for government policy on pensions and retirement age.

To obtain estimates of the changes in employment status, calibration is used to assign an appropriate weight to each sample member. Extreme weights are undesirable here, since that could lead to certain flow rates being over-estimated if certain sample members dominate. Much time is spent in designing the survey and sampling scheme to ensure that the sample is as representative as possible of the true population. Allowing weights to move close to 0 means that the corresponding sample member's contribution to the survey is removed. It would, effectively, have not been worth the cost of interviewing them and observing their characteristics, since they contribute very little to the subsequent estimates. This argument can also be applied to negative weights.

Therefore, taking all of this into account, the aim is to estimate employment flows such that

1. There is a close match between the sample estimates and known population totals;

2. There are non-extreme weights, i.e. not too large so that sample members dominate, and not too small or negative so that sample members are effectively unimportant to the estimates; and

3. The estimate of the flows is reliable, in a sense that to be defined later.

To begin, all possible combinations of algorithms and functions that have been introduced throughout this chapter shall be considered. This gives the following five cases:

1. Algorithm 1a for function $\phi^{(Q)}$ with no constraints;
2. Algorithm 1 for function $\phi^{(R)}$ with non-negativity constraints;
3. Algorithm 2 (and 2') for function $\phi^{(Q)}$ with general constraints;
4. Algorithm 2 (and 2') for function $\phi^{(R)}$ with general constraints; and
5. Algorithm 1 for function $\phi^{(L)}$ for general constraints.

For this example, general constraints are taken to be $l_i$=0.5 and $u_i$=2.4 for all $i = 1, \ldots, n$.

In Tables 7, 8 and 9 convergence of the algorithms is considered in all five cases listed above when using the Newton-Raphson, $g$-weights and identity matrix forms of $H^{(s)}$ respectively. The number of iterations (Iter), the minimum and maximum values of the $g$-weights obtained, as well as the mean, standard deviation (SD), coefficient of variation (CoV), skewness (Skew.), and kurtosis (Kurt.) of the weights are given. The 1st-percentile (1st %), the median (med), and the 99th-percentile (99th %) of the weights are also given in each case.

| $\phi$ | Constr. | Iter | Min | Max | Mean | SD | CoV | 1st-% | Med. | 99th-% |
|---|---|---|---|---|---|---|---|---|---|---|
| $\phi^{(Q)}$ | No | 1 | -0.087 | 3.173 | 0.989 | 0.491 | 49.629 | 0.213 | 0.910 | 2.428 |
| $\phi^{(R)}$ | Nonneg | 4 | 0.305 | 4.849 | 0.990 | 0.499 | 50.479 | 0.419 | 0.892 | 2.572 |
| $\phi^{(Q)}$ | Gen. | 5 | 0.500 | 2.400 | 0.990 | 0.498 | 50.329 | 0.500 | 0.887 | 2.400 |
| $\phi^{(R)}$ | Gen. | | | | | No convergence | | | | |
| $\phi^{(L)}$ | Gen. | 6 | 0.502 | 2.399 | 0.990 | 0.505 | 50.981 | 0.509 | 0.837 | 2.367 |

Table 7: Table comparing convergence properties of the calibrated $g$-weights using the Newton-Raphson version of $H^{(s)}$

Observe that there are negative $g$-weights for the function $\phi^{(Q)}$ with no constraints. There were 6 negative weights in this case. This is undesirable since sample members should not be under-represented in the estimates. Use of the raking function with non-negativity constraints has resulted in $g$-weights as large as 4.85. This is undesirable since individual sample members should not dominate the estimates.

| $\phi$ | Constr. | Iter | Min | Max | Mean | SD | CoV | 1st % | Med. | 99th-% |
|---|---|---|---|---|---|---|---|---|---|---|
| $\phi^{(Q)}$ | No | 1 | -0.087 | 3.173 | 0.989 | 0.491 | 49.629 | 0.213 | 0.910 | 2.428 |
| $\phi^{(R)}$ | Nonneg | 4 | 0.305 | 4.849 | 0.990 | 0.499 | 50.479 | 0.419 | 0.892 | 2.572 |
| $\phi^{(Q)}$ | Gen. | 15 | 0.500 | 2.400 | 0.989 | 0.4983 | 50.329 | 0.500 | 0.887 | 2.400 |
| $\phi^{(R)}$ | Gen. | | | | No convergence | | | | | |
| $\phi^{(L)}$ | Gen. | 75 | 0.502 | 2.399 | 0.990 | 0.505 | 50.979 | 0.509 | 0.837 | 2.367 |

Table 8: Table comparing convergence properties of the calibrated $g$-weights using the $g$-weights version of $H^{(s)}$

| $\phi$ | Constr. | Iter | Min | Max | Mean | SD | CoV | 1st % | Med. | 99th-% |
|---|---|---|---|---|---|---|---|---|---|---|
| $\phi^{(Q)}$ | No | 1 | -0.087 | 3.173 | 0.989 | 0.491 | 49.629 | 0.213 | 0.909 | 2.428 |
| $\phi^{(R)}$ | Nonneg | | | | No convergence | | | | | |
| $\phi^{(Q)}$ | Gen. | 5 | 0.500 | 2.400 | 0.990 | 0.498 | 50.329 | 0.500 | 0.887 | 2.400 |
| $\phi^{(R)}$ | Gen. | | | | No convergence | | | | | |
| $\phi^{(L)}$ | Gen. | 55 | 0.502 | 2.399 | 0.990 | 0.505 | 50.978 | 0.509 | 0.837 | 2.367 |

Table 9: Table comparing convergence properties of the calibrated $g$-weights using the identity matrix version of $H^{(s)}$

Observe that Algorithm 2 for $\phi^{(R)}$ with general constraints failed to converge (after running the algorithm for 100,000 iterations). The general constraints $l_i = 0.3$ and $u_i = 4$ were required so that Algorithm 2 converged in this case. In practice, the general constraints for the raking function need to be less 'severe' than for the quadratic or raking functions, in the sense of a smaller lower bound and/or a larger upper bound. This is due to the nature of the derivative of $\phi^{(R)}$ (as plotted in Figure 1(b)). The resulting $h$-function is such that its domain is smaller than for the quadratic and logit functions, despite having the same range.

There are several weights at the bounds in the case of the quadratic function, since the minimum and 1st-percentiles, and maximum and 99th-percentile are equal to the lower and upper bounds, respectively. In contrast, the minimum value of the $g$-weights for the logit function is greater than the lower bound, and the maximum $g$-weight is less than the upper bound.

Observe that the cases of the quadratic function with no constraints and the raking function with non-negative constraints lead to the same results as in Table 7. However, convergence for both the quadratic and logit functions with general constraints took more iterations than in the case of the Newton-Raphson form

of $H^{(s)}$. The algorithm has converged to the same place and the solutions are virtually identical in both cases.

In this case, the quadratic function with no constraints gives the same results as in Table 7 and Table 8. The quadratic function with general constraints converged in the same number of iterations as for the Newton-Raphson method considered in Table 7, since the matrices $H^{(s)}$ are equivalent in both cases. However, the algorithm failed to converge for the raking function in both the non-negativity and general constraint cases. The logit function with general constraints took longer to converge than for the Newton-Raphson form of the matrix $H^{(s)}$ considered in Table 7; however, using the identity matrix form of $H^{(s)}$ took fewer iterations to converge than for the $g$-weights form of $H^{(s)}$ considered in Table 8.

For a general discussion on measuring numerical complexity of an optimization problem see [38, 68, 69]. For a discussion on choosing test functions for optimization problems see [67].

In Figure 12, a box-plot of the calibrated weights considered in Table 7 is presented. The calibrated weights for the quadratic and logit functions using the general constraints $l_i = 0.3$ and $u_i = 3$ are also included (the raking function with general constraints failed to converge in this case).

In Figure 13, histograms of the weights obtained using Algorithm 2 for function $\phi^{(Q)}$ (Figure 13(a)) and Algorithm 1 for function $\phi^{(L)}$ (Figure 13(b)) in the case of the general constraints $l_i = 0.5$ and $u_i = 2.4$ are plotted. These correspond to cases 5 and 3, respectively, in Figure 12. From Figure 13(a), observe that many of the weights have been projected to the boundaries. In contrast, Figure 13(b) shows that many $g$-weights approach, but do not reach, the bounds. This supports our comments from Example 2 in Section 3.4.

In Figure 14, histograms of the weights using Algorithm 2 for function $\phi^{(Q)}$ (Figure 14(a)) and Algorithm 1 for function $\phi^{(L)}$ (Figure 14(b)), both in the case of the general constraints $l_i = 0.3$ and $u_i = 3$ are plotted. These correspond to cases 6 and 4, respectively, in Figure 12. The histogram in Figure 14(b) shows that there are fewer weights with values at the lower and upper bounds. Contrast this

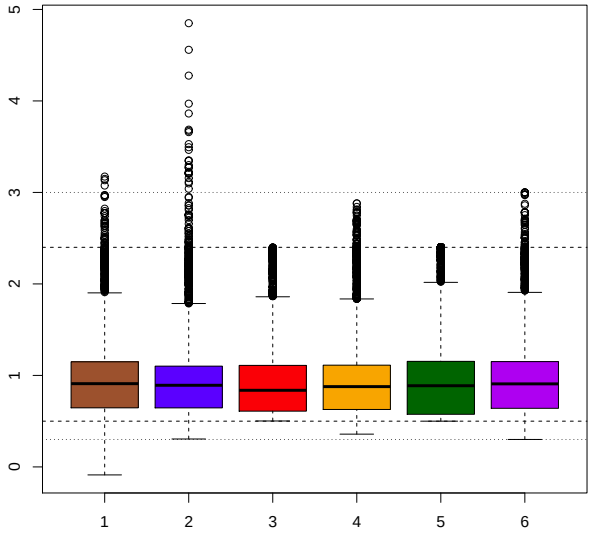



Figure 12: Box-plot of $g$-weights for: *1.* $\phi^{(Q)}$ with no constraints, *2.* $\phi^{(R)}$ with non-negativity constraints, *3.* $\phi^{(L)}$ with general constraints ($l = 0.5$ and $u = 2.4$), *4.* $\phi^{(L)}$ with general constraints ($l = 0.3$ and $u = 3$), *5.* $\phi^{(Q)}$ with general constraints ($l = 0.5$ and $u = 2.4$), and *6.* $\phi^{(Q)}$ with general constraints ($l = 0.3$ and $u = 3$)

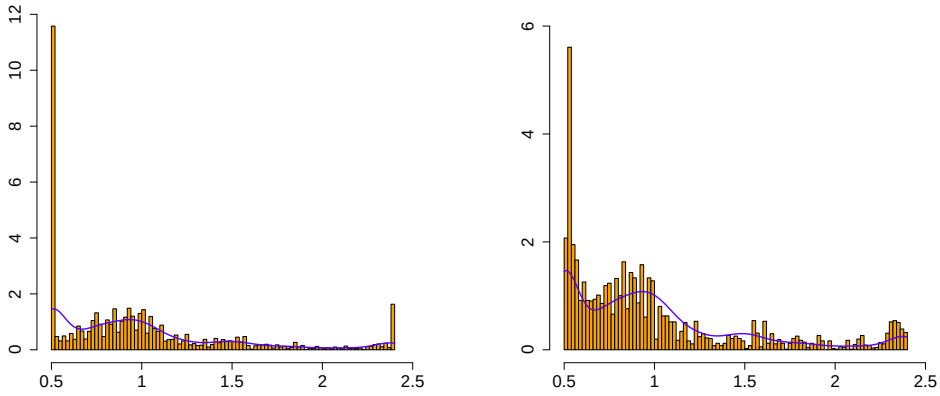
to Figure 14(a), where the histogram shows that there are many weights with values at the lower and upper bounds.

For the histograms in Figure 13, most of the weights are at or near the boundaries, with few weights in between. However, as the difference between the bounds is increased, fewer weights move towards these bounds. The resulting distribution is uni-modal or bi-modal depending on the nature of the imposed bounds.

This example can be summarised as follows:

**Algorithm 1a for function $\phi^{(Q)}$ with no constraints** All three forms of $H^{(s)}$ are equivalent and the algorithm gives the same solution.

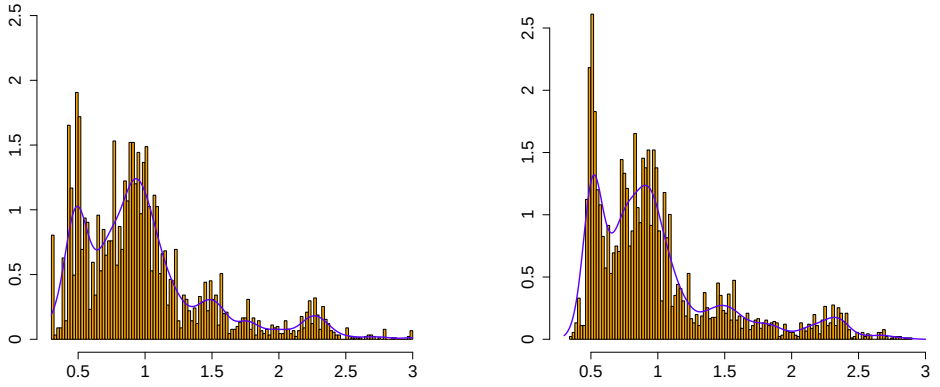
**Algorithm 1 for function $\phi^{(R)}$ with non-negativity constraints** The Newton-Raphson and $g$-weights form of the matrix $H^{(s)}$ are the same and the algorithms




(a) $g$-weights using Algorithm 2 with $\phi^{(Q)}$

(b) $g$-weights using Algorithm 1 with $\phi^{(L)}$

Figure 13: Histogram *(orange)* and density plot *(blue line)* of the calibrated weights for the truncated quadratic function $\phi^{(Q)}$ and the logit function $\phi^{(L)}$ for the general constraints $l_i = 0.5$ and $u_i = 2.4$




(a) $g$-weights using Algorithm 2 with $\phi^{(Q)}$

(b) $g$-weights using Algorithm 1 with $\phi^{(L)}$

Figure 14: Histogram *(orange)* and density plot *(blue line)* of the calibrated weights for the truncated quadratic function $\phi^{(Q)}$ and the logit function $\phi^{(L)}$ for the general constraints $l_i = 0.3$ and $u_i = 3$

converge to the same solution in the same number of iterations for both cases. However, the algorithms failed to converge in the case of the identity matrix.

**Algorithm 2 (and 2') for function $\phi^{(Q)}$ with general constraints** The algorithm converged in the fewest iterations in the case of the Newton-Raphson and identity forms of $H^{(s)}$. The algorithm converged to the same solution using the $g$-weights form of $H^{(s)}$, but took more iterations to converge.

**Algorithm 2 (and 2') for function $\phi^{(R)}$ with general constraints** There was no convergence for any case of $H^{(s)}$. This is likely to be due to the general constraints being too restrictive for this choice of function.

**Algorithm 1 for function $\phi^{(L)}$ for general constraints** Converged in the fewest iterations for the Newton-Raphson version of $H^{(s)}$. The identity matrix version of $H^{(s)}$ was the second fastest in terms of the number of iterations, with the $g$-weights version of $H^{(s)}$ requiring the most iterations to converge.

A major criticism of Algorithm 2 is that, following the projections of the weights using Algorithm 2', the vector $\Lambda$ is not updated to reflect this projection. Therefore, the same vector $\Lambda$ is used before and after the projections. It is not possible to determine a suitable vector $\Lambda$ for the updated weights $G$. Recall that $g_i = h(\mathbf{a}_i\Lambda)$, for $i = 1, \ldots, n$. This creates $n$ equations in $m$ unknowns (namely $\lambda_1, \ldots, \lambda_m$). Recall that a system of linear equations with more equations than unknowns (usually) has no solution, since the system is overdetermined (see for example [41]).

## 3.5 Other Algorithms

Whilst the algorithms that are arguably most commonly used in the calibration software have been considered in this section, there are several algorithms that have not been considered. A brief summary of some of these methods is presented in this section.

**Scale Modified Quadratic** The scale modified quadratic algorithm uses projections to satisfy the calibration constraints $A'G = T$ at each iteration, continuing

until the range restrictions $L \leq G \leq U$ are met to within a pre-specified accuracy. The algorithm is applied only in the case of function $\phi^{(Q)}$ with general constraints. This algorithm is attributed to [29]. The method is outlined in [56] (see Method 3) with further information in Section 2.2 of [46]. This algorithm is used in the calibration software BASCULA (see Section 3.6.2 for further information).

**Shrinkage Minimization Method** The shrinkage minimization method uses a similar algorithm to the scaled modified quadratic algorithm, but is not considered here as it is not used by any of the packages considered in this chapter. See Method 4 of Singh and Mohl [56] and Section 2.4 of Rao and Singh [46] for more information on the shrinkage minimization method.

**Projection Method Algorithm** This algorithm uses a method attributed to Han [26] with details outlined by Estevao in [21]. The algorithm is only used for the case of the quadratic function $\phi^{(Q)}$ with general constraints.

*Suppose $l$ and $u$ are given. Choose parameters $\alpha$ and $\beta$ such that $0 \leq \alpha, \beta \leq 1$ and set $l' = \alpha l + 1 - \alpha$, $u' = \alpha u + 1 - \alpha$. Set $H^{(s)} = diag(q_k^{(s)}), k = 1, \ldots, n$. Define the following $n$-vectors:*

1. $\xi^{(s)}$ with entries $\xi_k^{(s)} = \begin{cases} (g_k^{(s)} - 1)/(l' - 1) & \text{if } g_k^{(s)} \leq 1; \\ (g_k^{(s)} - 1)/(u' - 1) & \text{otherwise.} \end{cases}$

2. $Q^{(s)}$ with entries $q_k^{(s)} = \begin{cases} 1 & \text{if } \xi_k^{(s)} < 1/2; \\ 1 - \beta(\xi_k^{(s)} - 1/2)^2 & \text{if } 1/2 \leq \xi_k^{(s)} < 1; \\ (1 - \beta/4)/\xi_k^{(s)} & \text{if } \xi_k^{(s)} \geq 1. \end{cases}$ Note that $Q^{(0)} = \mathbf{1}$.

3. $Q^{[s+1]}$ with entries $q_k^{[s+1]} = q_k^{[s]} q_k^{(s+1)}$.

For $s = 0, 1, 2, \ldots$.

1. Compute $G^{(s+1)} = \mathbf{1} + Q^{[s]} A(A' H^{(s)} A)(T - A'\mathbf{1})$;

2. Repeat until RRs are satisfied or maximum number of iterations met.

This algorithm is used in Statistics Canada's GES software (see Section 3.6.2 for further details).

The algorithms presented in this section generally give the same results as the other algorithms presented in the previous sections. Investigation with the projection method algorithm gave results that were always identical to those for Algorithms 2 and 2' when using the quadratic function with general constraints. Authors such as Nieuwenbroek and Boonstra [40] have made comparisons between the methods presented in this section and the more standard calibration algorithms outlined earlier. In general, their findings showed that the algorithms lead to the same solutions. We shall therefore not give any further consideration to the algorithms described in this section.

## 3.6 Calibration Software

Calibration is a task performed on a day-to-day basis in statistical offices throughout the world. To perform the calibration, standard software packages are typically used. The purpose of this chapter is to provide a critical analysis of some of the most famous packages. The software used is arguably outdated, and the optimization algorithms used are often unreliable. In this chapter, only algorithms for hard calibration are considered, which is the main case in practice, but the discussion can be easily extended to soft calibration. Algorithms for soft calibration shall be described further in Chapter 5.

In the next section, a critical analysis of the various software packages that perform calibration, along with the algorithms and calibration functions they implement, is given.

### 3.6.1 Summary of the Calibration Packages

Table 10 gives a summary of some of the packages that implement the calibration algorithms presented in this chapter. In the table below, the three functions $\phi$ presented in Section 3.1 are referred to, namely the quadratic function $\phi^{(Q)}$, the

| Package | Program | Functions | Constraints | Matrix $H$ |
|---|---|---|---|---|
| CALIB | R | $\phi^{(Q)}$ | (a) and (c) | Identity Matrix |
| | (sampling) | $\phi^{(R)}$ | (b) | $g$-weights Matrix |
| | | $\phi^{(L)}$ | (c) | $g$-weights Matrix |
| CALIBRATE | R | $\phi^{(Q)}$ | (a) and (c) | Newton-Raphson |
| | (survey) | $\phi^{(R)}$ | (b) and (c) | Newton-Raphson |
| | | $\phi^{(L)}$ | (c) | Newton-Raphson |
| ReGenesees | R | $\phi^{(Q)}$ | (a) and (c) | Newton-Raphson |
| | | $\phi^{(R)}$ | (b) | Newton-Raphson |
| | | $\phi^{(L)}$ | (c) | Newton-Raphson |
| CALMAR | SAS | $\phi^{(Q)}$ | (a) and (c) | Newton-Raphson |
| CALMAR 2 | | $\phi^{(R)}$ | (b) | Newton-Raphson |
| | | $\phi^{(L)}$ | (c) | Newton-Raphson |
| g-CALIB-S | SPSS | $\phi^{(Q)}$ | (a) and (c) | Newton-Raphson |
| | | $\phi^{(R)}$ | (b) | Newton-Raphson |
| | | $\phi^{(L)}$ | (c) | Newton-Raphson |
| GES | SAS | $\phi^{(Q)}$ | (a) and (c) | Projection Method Algorithm |
| BASCULA | Blaise | $\phi^{(Q)}$ | (a) and (c) | Scale Modified Quadratic |

Table 10: Summary of the main calibration packages and the algorithms they implement

raking function $\phi^{(R)}$, and the logit function $\phi^{(L)}$. For the various functions, the packages implement the different cases of the $g$-weight constraints outlined in Section 2.4. In Table 10, each of the constraint cases indicated by the letters (a), (b), and (c) correspond to the labels used in the list given in Section 2.4. The case (a) refers to no constraints, case (b) refers to non-negativity constraints, and case (c) refers to general constraints. Three versions of the matrix $H^{(s)}$ as introduced in Section 3.2.5 are also referred to. Recall that the three versions are the Newton-Raphson matrix, identity matrix, and matrix with $g$-weights on the diagonal ($g$-weights matrix).

### 3.6.2 Details of the Calibration Packages

This section expands on the information presented in Table 10 of Section 3.6.1. All packages give the option to use Algorithm 1a (see Section 3.3.3) for the quadratic function with no constraints. An overview of each of the programs and the algorithms they implement is given.

**Calib** This is a function that is part of the 'sampling' package [61] in R. It uses Algorithm 1 for the functions $\phi^{(L)}$ and $\phi^{(R)}$, and Algorithm 2 (and 2') for the function $\phi^{(Q)}$. The algorithm uses the $g$-weights form of $H^{(s)}$ for the logit and raking functions and the identity matrix form of $H^{(s)}$ in the case of the quadratic function.

**Calibrate** This is an R function contained within the 'survey' package [36]. The package has the options to use Algorithm 1 for the functions $\phi^{(L)}$ and $\phi^{(R)}$ in the case of general constraints and non-negativity constraints, respectively, and Algorithm 2 (and 2') for the functions $\phi^{(Q)}$ and $\phi^{(R)}$ in the case of general constraints. The Newton-Raphson form of $H^{(s)}$ is implemented in all cases. There is the option for the user to input his/her own calibration functions; however, this requires stating the function $h$, i.e. the inverse of the derivative of the function $\phi$.

**ReGenesees** This is an R package [65] developed by the Italian Statistical Office, ISTAT, that implements the function ecalibrate. The user may choose from the quadratic, raking, and logit functions. Algorithm 1 is performed for functions $\phi^{(L)}$ and $\phi^{(R)}$ in the case of general constraints and non-negativity constraints, respectively, whilst Algorithms 2 (and 2') are used for the quadratic and raking functions $\phi^{(Q)}$ and $\phi^{(L)}$ with general constraints. The Newton-Raphson form of the matrix $H^{(s)}$ is implemented for all functions.

**CALMAR** The software CALMAR (CALibration of MARgins) is used by the Office for National Statistics in the UK, the Central Statistical Office in Ireland and many other statistical offices throughout the world. The package was developed by Sautory [53] at the French National Institute for Statistics and Economic Studies (INSEE). The software uses a SAS Macro [54] to perform Algorithm 1 for functions $\phi^{(L)}$ and $\phi^{(R)}$ in the case of general constraints and non-negativity constraints, respectively, as well as Algorithms 2 (and 2') for function $\phi^{(Q)}$ with general constraints. The Newton-Raphson form of $H^{(s)}$ is used for all functions.

**CALMAR2** This is a modified version of the SAS macro CALMAR introduced above. Sautory [33] enhanced several aspects of the original CALMAR code, allowing the user to perform simultaneous calibration at different levels of a survey, and use generalized calibration adjustment for total non-response (see [55] for further information). CALMAR2 also includes a new function referred to as the hyperbolic sine function. It is not widely used in practice, and so has not been discussed in this chapter. CALMAR2 is used at INSEE, as well as several other statistical offices worldwide. With the exception of the new hyperbolic sine function (which is not discussed here), the functions and algorithms implemented are as described for CALMAR.

**g-CALIB-S** This is an SPSS package developed at Statistics Belgium. The package is very similar to CALMAR, in that Algorithm 1 may be used for functions $\phi^{(L)}$ and $\phi^{(R)}$ in the case of general constraints and non-negativity constraints, respectively, as well as Algorithms 2 (and 2') for function $\phi^{(Q)}$ with general constraints. The Newton-Raphson form of $H^{(s)}$ is used for all functions. This package is well documented in [62].

**GES** The Generalized Estimation Software (GES) was developed by Statistics Canada, and uses a projection method algorithm (see Section 3.5) for the quadratic function $\phi^{(Q)}$ with general constraints (see [22] for a more detailed discussion). The package is used by the Office for National Statistics (ONS) in the analysis of quarterly Labour Force Survey (LFS) datasets. Note, however, that for the longitudinal five-quarterly datasets as considered in Section 3.4, the ONS currently uses CALMAR rather than GES.

The paper of [10] compares the GES algorithm with a so-called new algorithm. This algorithm is equivalent to Algorithm 2 (and 2'). It is shown in [10] that the "new" algorithm converges in fewer iterations than the GES algorithm. They also show that, when the bounds are tightened, the time taken for the 'new' algorithm to converge decreases. This is a consequence of the algorithm setting more weights to the bounds at earlier iterations.

It is argued in [10] that an 'obvious' advantage of the CALMAR algorithm is that it gives a solution that lies entirely within or on the boundary values. Therefore, the bounds will be satisfied exactly. However, for the projection method algorithm used by GES, the bounds are not met exactly and are only satisfied to within the convergence level specified by the user. Despite this, it is argued that when the calibration problem with bounds is not solvable, the projection method algorithm is better than the 'new' algorithm, in that the projection method algorithm will give an approximate solution. However, caution should be taken here as the algorithm may not have given a valid approximation to the solution of the calibration problem in this case.

It could also be argued that soft calibration is a useful method of obtaining an approximate solution when the hard calibration problem cannot be solved. See Section 5 of [15] for further information regarding soft calibration.

**BASCULA** This program implements the scale modified quadratic algorithm attributed to [29] for the function $\phi^{(Q)}$ with general constraints. This algorithm is equivalent to Method 3 considered in [56]. The package was developed by Statistics Netherlands and is well documented in the Bascula 4.0 User Guide [40]. There has been criticism of the convergence properties of this algorithm (and hence the BASCULA package), see, for example, the technical paper [12].

## 3.7 Summary

In this chapter, existing calibration algorithms that are implemented by many standard software packages have been described. The exact mathematical formulation of these algorithms cannot be found in existing literature. The behaviour and convergence properties of these algorithms has been explored and a critical analysis of existing software packages given.

A critical analysis of existing calibration algorithms and software packages has been provided. Some of these algorithms are more efficient than others, due to the form of a matrix that is used within the algorithms, referred to as $H^{(s)}$ throughout

this chapter. The impact of the various forms of this matrix has been described, and the recommendation is to use the Newton-Raphson form of the matrix since this is the form that is derived theoretically. The matrix with $g$-weights on the diagonal generally performed the worst, and although this generally gives a stable solution when the Newton-Raphson method does not, use of the identity matrix generally performs better.

This chapter has predominantly focused on the algorithms that are used in existing software packages. However, there is scope to extend these algorithms to other calibration functions. In the next chapter, the choice of the calibration functions shall be discussed in more detail. The benefits and drawbacks of various calibration functions, including those presented in this chapter, shall be further explored.

# 4 Functions for Calibration

In this chapter, a class of new calibration functions is proposed that have several desirable properties, including satisfying necessary range restrictions for the weights. The impact of these new functions on the calibrated weights shall be explored.

## 4.1 Introduction

In Chapter 2, the calibration problem was introduced as an optimization problem. Recall that the hard calibration problem can be described as

$$\Phi(G) \to \min_{G \in \mathbb{G}}, \text{ where } \mathbb{G} = \{G : L \leq G \leq U \text{ and } A'G = T\}. \tag{17}$$

Recall also that the soft calibration problem considered in this thesis is

$$\Phi(G) + \Psi(A'G, T) \to \min_{G \in \mathbb{G}}, \text{ where } \mathbb{G} = \{G : L \leq G \leq U\}. \tag{18}$$

In both cases,

$$\Phi(G) = \Phi(g_1, \ldots, g_n) = \sum_{i=1}^{n} q_i \phi_i(g_i)\,. \tag{19}$$

Here $\phi$ is a specified calibration function and $q_1, \ldots, q_n$ are given non-negative numbers. In the majority of applications $q_i = d_i$ for all $i$; it is assumed that $q_i = d_i$ throughout this chapter. The vectors $L$ and $U$ are $n$-vectors of lower and upper bounds for the $g$-weights $G$, respectively, $A$ is a known matrix derived from the sample observations, and $T$ is an $m$-vector of known population totals.

In this chapter, only consider choices of the function $\phi$ in $\Phi$ are considered. The function $\Psi$ will be discussed in more detail in Chapter 5.

## 4.2 Choice of the function $\phi$

In this section, the choice of the functions $\phi_i$ in (19) is discussed. See Section 4.3 for examples of calibrated weights obtained using different forms of functions $\phi_i$. The function $\phi_i : (l_i, u_i) \to \mathbb{R}_+$ needs to satisfy the following:

(i) $\phi_i(g) \geq 0$ for all $g \in (l_i, u_i)$,

(ii) $\phi_i(1) = 0$,

(iii) $\phi_i$ is twice continuously differentiable and strictly convex.

The function $\phi_i$ does not have to be defined outside the open interval $(l_i, u_i)$. If all $\phi_i$ satisfy conditions (i)-(iii) then the function $\Phi$ defined in (19) satisfies the conditions (I)-(IV) formulated in Section 2.5.

Since these functions are chosen in the same manner for all $i$, the subscript $i$ will be dropped and the function $\phi_i$ will be denoted simply by $\phi$. Correspondingly, the lower and upper bounds $l_i$ and $u_i$ for the $g$-weights $g_i$ will be denoted by $l$ and $u$, respectively.

As mentioned in Chapter 1, the functions $\phi$ are often referred to as 'distance' functions in the classical calibration literature, see for example [8] and [19]. However, it should be noted that several of the functions $\phi^{(1)}$ to $\phi^{(8)}$ do not satisfy the triangle inequality. Therefore, these functions are better thought of as objective functions or divergence measures (see [44] for further discussion of divergence measures).

It is important to distinguish between the following two types of functions $\phi$:

**Type I** $\phi(g)$ is defined for all $g$ either in $\mathbb{R}$ or $\mathbb{R}_+ = (0, \infty)$ and does not depend on $l$ and $u$.

**Type II** $\phi(g)$ is defined for $g \in (l, u)$ but not outside the interval $[l, u]$. The functional form of $g$ depends on $l$ and $u$ and hence the notation $\phi(g; l, u)$ will be used for the functions $\phi$ of this type.

The authors of the classical papers [19] and [20] suggest six choices for the function $\phi$. Five of these are Type I functions and are as follows:

(1) $\phi^{(1)}(g) = (g-1)^2$,

(2) $\phi^{(2)}(g) = g \ln g - g + 1$,

(3) $\phi^{(3)}(g) = (\sqrt{g} - 1)^2$,

(4) $\phi^{(4)}(g) = -\ln g + g - 1$,

(5) $\phi^{(5)}(g) = (g-1)^2 / g$.

The function $\phi^{(1)}$ is simply quadratic; in the literature on calibration it is usually referred to as the 'chi-square' function (see for example [45], equation (2.10)). It is by far the most popular in practice. The function $\phi^{(2)}$ is often referred to as the multiplicative or raking function (see for example [2]).

Many authors consider solving optimization problem (17) without the constraint $L \leq G \leq U$. However, in this case using the function $\phi^{(1)}$ in the optimization may lead to extreme and negative weights. Whilst the function $\phi^{(2)}$, by the nature of its domain, only permits non-negative values for the optimized weights, the weights may still take very large values. This also applies to functions $\phi^{(3)}$, $\phi^{(4)}$ and $\phi^{(5)}$. The functions $\phi^{(3)}$, $\phi^{(4)}$ and $\phi^{(5)}$ have received much less attention in the literature on calibration.

The above criticism of the functions $\phi^{(1)}$–$\phi^{(5)}$ can be extended to all functions of Type I. Note that if functions $\phi$ of Type I are used then the optimization problem (17) is an optimization problem with many variables and many constraints (recall that $n$ is typically very large).

To overcome the issue of negative and extreme weights, the authors of [19] proposed the introduction of range restrictions on the weights. Recall that this requires defining two vectors $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$ such that the $g$-weights satisfy $l_i \leq g_i \leq u_i$ for all $i = 1, \ldots, n$. Equivalently, the calibrated weights $W = (w_1, \ldots, w_n)$ must satisfy the constraint $l_i d_i \leq w_i \leq u_i d_i$ for all $i = 1, \ldots, n$.

The authors of [19] proposed two approaches to this problem. The first approach is to run a constrained optimization problem, such that the objective function is any calibration function $\phi$ of Type I. The second approach is to define suitable calibration functions that incorporate the constraints within the function definition, i.e. defining a function that can only take values within the required range. In order to define an appropriate function, the function (in terms of the $g$-weights) should take its minimum value is at 1 and that increases rapidly as $l_i$ and $u_i$ are approached. These are Type II functions.

Let us consider three functions $\phi$ of Type II:

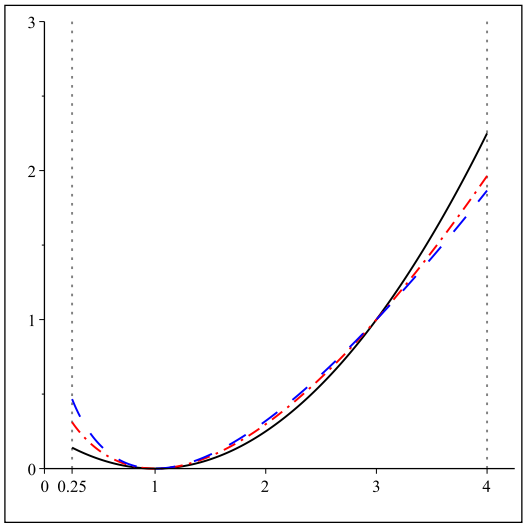
$$\begin{aligned}
\phi^{(6)}(g;l,u) &= (g-l)\ln\left(\frac{g-l}{1-l}\right)+(u-g)\ln\left(\frac{u-g}{u-1}\right), \\
\phi^{(7)}(g;l,u) &= (1-l)\ln\left(\frac{1-l}{g-l}\right)+(u-1)\ln\left(\frac{u-1}{u-g}\right), \qquad (20)\\
\phi^{(8)}(g;l,u,\alpha) &= \frac{(g-1)^2}{[(u-g)(g-l)]^{\alpha}}, \quad \alpha>0\,. \qquad (21)
\end{aligned}$$

The shape of several functions $\phi$ are illustrated in Figures 15–17. In all these figures, the values $l = 1/4, u = 4$ are used and all the functions are plotted in the interval $(l,u) = (\frac{1}{4}, 4)$, despite some of the functions are defined on a larger domain.

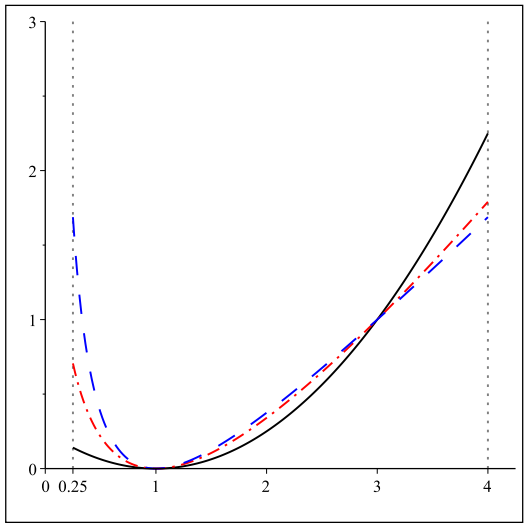
As our intention in this section is illustrating shapes of the possible calibration functions $\phi$. Thus, scaled versions of these functions are plotted using appropriate multiples (so that different functions become visually comparable). In Figure 15, each of the Type I functions $c_k\phi^{(k)}(g)$, $k = 1,\ldots,5$, are plotted with the constants $c_k$ chosen so that $c_k\phi^{(k)}(3) = 1$.

In Figure 16, the functions $c_1\phi^{(1)}(g)$, $c_6\phi^{(6)}(g;\frac{1}{4},4)$, $c_7\phi^{(7)}(g;\frac{1}{4},4)$ and $c_{8,1}\phi^{(8)}(g;\frac{1}{4},4,1)$ are plotted with the constants $c_1$, $c_6$, $c_7$ and $c_{8,1}$ chosen so that $c_1\phi^{(1)}(3) = 1$, $c_k\phi^{(k)}(3;\frac{1}{4},4) = 1$ for $k = 6, 7$ and $c_{8,1}\phi^{(8)}(3;\frac{1}{4},4,1) = 1$.

In Figure 17, function $\phi^{(8)}$ is plotted for various values of the parameter $\alpha$. In Figure 17(a), the constants $c_{8,\alpha}$ are chosen so that $c_{8,\alpha}\phi^{(8)}(3;\frac{1}{4},4,\alpha) = 1$. In Figure 17(b), the constants $c_{8,\alpha}$ are chosen so that $c_{8,\alpha}\phi^{(8)}(\frac{1}{2};\frac{1}{4},4,\alpha) = \frac{1}{2}$.

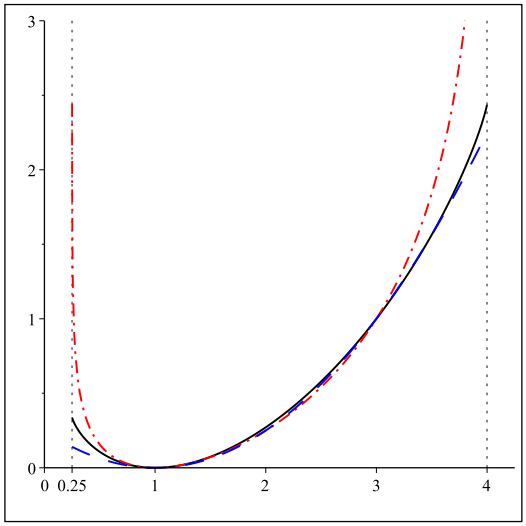



(a) $\phi^{(1)}$ (line), $\phi^{(2)}$ (dot-dash) and $\phi^{(3)}$ (dash)

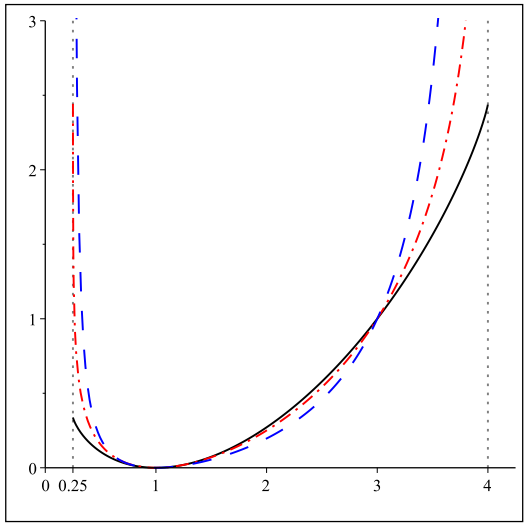



(b) $\phi^{(1)}$ (line), $\phi^{(4)}$ (dot-dash) and $\phi^{(5)}$ (dash)

Figure 15: Calibration functions of Type I scaled so that $c_k\phi^{(k)}(3) = 1$, $k = 1, ..., 5$.



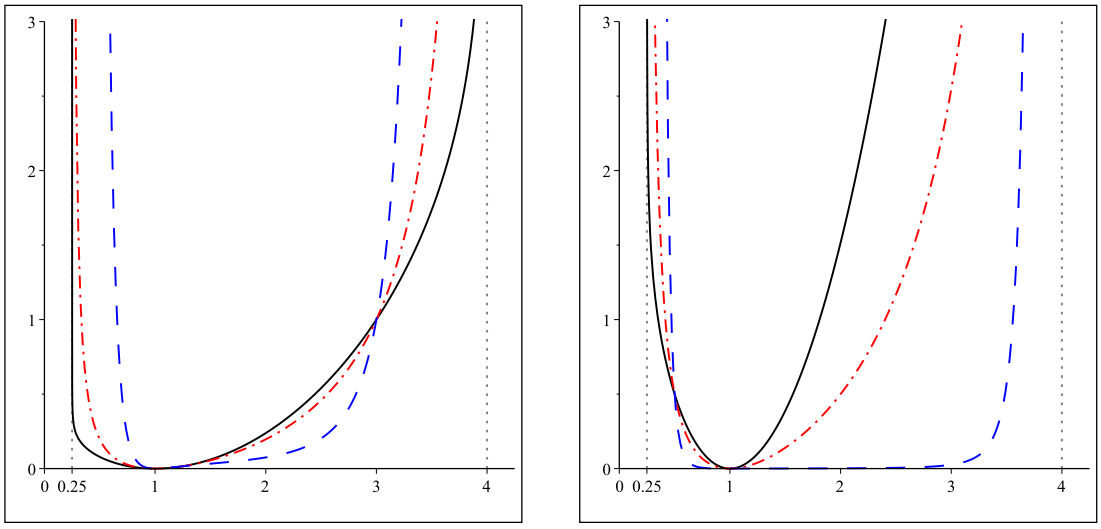

(a) $\phi^{(6)}$ (line) and $\phi^{(7)}$ (dot-dash) and $\phi^{(1)}$ (dash)




(b) $\phi^{(6)}$ (line), $\phi^{(7)}$ (dot-dash) and $\phi^{(8)}$ with $\alpha = 1$ (dash)

Figure 16: Functions $\phi^{(1)}$ $\phi^{(6)}$, $\phi^{(7)}$ and $\phi^{(8)}$ scaled so that $c_1\phi^{(1)}(3) = 1$ and $c_k\phi^{(k)}(3; \frac{1}{4}, 4) = 1$, $k = 6, 7$ and $c_{8,1}\phi^{(8)}(3; \frac{1}{4}, 4, 1) = 1$.

The function $\phi^{(6)}$ is defined on the closed interval $g \in [l, u]$ so that by continuity $\phi^{(6)}(l; l, u) = (u - l) \ln \frac{u-l}{u-1}$ and $\phi^{(6)}(u; l, u) = (u - l) \ln \frac{u-l}{1-l}$. The function $\phi^{(6)}(g; l, u)$ is not defined outside the interval $[l, u]$. Using this function in (19) creates difficulties for the algorithms that optimize (19) because of discontinuity




(a) $\phi^{(8)}$ scaled so that $c_{8,\alpha}\phi^{(8)}(3;l,u,\alpha)=1$: $\alpha=0.2$ (line), $\alpha=1$ (dot-dash) and $\alpha=5$ (dash)

(b) $\phi^{(8)}$ scaled so that $c_{8,\alpha}\phi^{(8)}(\frac{1}{2};l,u,\alpha)=\frac{1}{2}$: $\alpha=0.2$ (line), $\alpha=1$ (dot-dash) and $\alpha=5$ (dash)

Figure 17: Function $\phi^{(8)}(g;l,u,\alpha)$ for various values of $\alpha$ with $l=1/4$ and $u=4$.

(and loss of convexity) of $\phi^{(6)}(g;l,u)$ at $g=l$ and $g=u$. A way around this is the use of constrained optimization algorithms but then the criticism above directed to Type I functions can be extended to the function $\phi^{(6)}$.

The functions $\phi^{(7)}(g;l,u)$ and $\phi^{(8)}(g;l,u,\alpha)$ are derived by us. These two functions are defined only in the open interval $g\in(l,u)$ and tend to infinity as $g$ tends to either $l$ or $u$. Both functions can be classified as interior penalty functions. The expression for the function $\phi^{(7)}$ has been derived by applying a suitable transformation (including taking a logarithm) to the density of the Beta-distribution on $[0,1]$. The convexity of the function $\phi^{(7)}$ follows from the expression for its second derivative:

$$\frac{\partial^2\phi^{(7)}(g;l,u)}{\partial g^2}=\frac{(u-l)\,(g^2-lu-2\,g+l+u)}{(g-l)^2\,(u-g)^2}=\frac{(u-l)\,[(g-1)^2+(u-1)(1-l)]}{(g-l)^2\,(u-g)^2}\,.$$

Since $0\le l<1<u\le\infty$, this second derivative is positive for all $g\in(l,u)$ so that the function $\phi^{(7)}(g;l,u)$ is convex. The analytic forms of the functions $\phi^{(6)}$ and $\phi^{(7)}$ are very similar, but the properties of the function $\phi^{(7)}$ are more attractive for the problem at hand than the properties of the function $\phi^{(6)}$.

For any $\alpha > 0$, the function $\phi^{(8)}$ has properties similar to the function $\phi^{(7)}$: it is defined in the open interval $g \in (l, u)$, it is convex in this interval, and it tends to infinity as $g \to l$ or $g \to u$. The function $\phi^{(8)}$ depends on an extra shape parameter $\alpha$, see Figure 17, so that the penalty for $g$ deviating from 1 can be adjusted by the user.

A very important special case of the function $\phi^{(8)}$ occurs when $\alpha = 1$:

$$\phi^{(8)}(g; l, u, 1) = \frac{(g-1)^2}{(u-g)(g-l)}\,. \tag{22}$$

The most attractive property of function $\phi^{(8)}$ is its invariance with respect to the change $g \leftrightarrow 1/g$ in the case $l = 1/u$ (which is a very common case in practice). Recall that $g = w/d$ is the ratio of the calibrated weight $w$ to the initial weight $d$ and therefore the multiplicative scale for measuring deviations of $g$ from 1 is the most appropriate. This means that it is very natural to penalize $g$ as much as $1/g$ for deviating from 1. Assuming $\alpha = 1$ and $l = 1/u$, then

$$\phi(g; u) = \phi^{(8)}(g; 1/u, u, 1) = \frac{(g-1)^2}{(u-g)(g-1/u)}.$$

For this function, $\phi(g; u) = \phi(1/g; u)$. This function possesses the additional property of equally penalizing $g$ and $1/g$.

## 4.3 Hard Calibration

In this section, the optimization problem (17) is considered, namely calibration with hard constraints. For several examples, the calibrated weights obtained using each of the functions considered in Section 4.2 shall be compared.

To solve the optimization problem (17), the 'solnp' function within the Rsolnp package in R (see [25]) is used. Using this software, it is possible to directly solve optimization problem (17) using the Augmented Lagrange Multiplier (ALM) method (see [30] for more details) for any choice of Type I or Type II function. For a comprehensive optimization software guide, see [39].

Recall that there are three choices for the vectors of lower and upper bounds, i.e. three choices for $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$, respectively. These are

(a) no constraints: $l_i = -\infty$ and $u_i = \infty$ for all $i$;

(b) non-negativity constraint: $l_i = 0$ and $u_i = \infty$ for all $i$;

(c) general constraints: $0 \leq l_i < 1 < u_i \leq \infty$.

There are many software packages that perform calibration using an iterative Newton method, see Chapter 3.3 for further information. Examples of the software packages include the 'calib' function within the sampling package in R (see [60]), the g-CALIB-S module within SPSS (see [62]) and the package CALMAR in SAS (see [19]). See Section 3.6 for more information about these and other calibration packages.

Many statistical offices throughout Europe use calibrated weights obtained via these packages. When comparing the weights obtained using direct optimization with the weights given by these packages, the weights obtained through direct optimization and using the calibration packages were usually the same to within computer error (despite the running time was in some cases very different). Some of the issues with the calibration packages has already been discussed in Chapter 3. For the remainder of this chapter, the calibration problem shall be solved using direct optimization by the ALM method.

To begin, let us consider an example adapted from [29] using data from [14]. In this example, the calibrated weights for various calibration functions are investigated, including an illustration of how Type I functions may lead to negative and extreme weights.

### 4.3.1 Example 1: Estimating the Population Total of 49 Cities

Consider the following example adapted from Huang and Fuller in [29] using data from Cochran in [14]. Throughout this example the units are in thousands of people. Suppose the population total of 49 cities in 1930 needs to be estimated. A sample of 12 of these cities is taken and needs to be weighted appropriately to

provide an estimate the population total from all 49 cities. For the 12 sampled cities, the number of people living in these cities in 1920 and 1930 is known. The size of the population from all 49 cities in 1920 is known to be 5054, i.e. $T = 5054$. In reality, the size of the population from all 49 cities in 1930 would be unknown. However, for this example it is known to be 6262. This value will be useful comparative purposes when comparing estimates of the total size of the 49 cities in 1930. The key information for this example is summarized in the following table.

| **Size of city in 1920** $(X)$ | **Size of city in 1930** $(Y)$ |
|---|---|
| 12 sample values known | 12 sample values known |
| Total size of population known (49 cities) | Total size of population to be estimated (49 cities) |

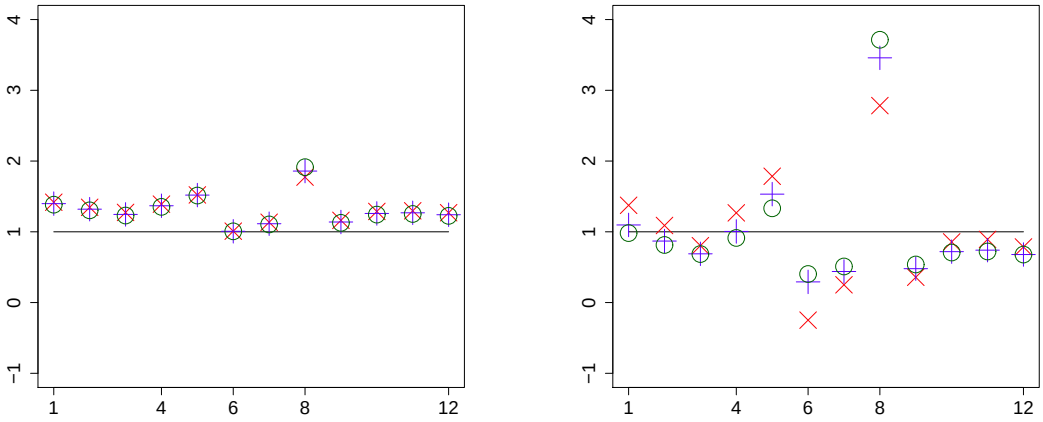
Table 11: Summary of the data available in Example 1

The initial vector of $g$-weights is $G = \mathbf{1}$ and the initial weights are taken to be $D = (49/12, 49/12, ..., 49/12)'$. These initial weights are derived using the classical Horvitz-Thompson estimator [28]. In practice, some adjustments are made to the initial weights $D$ to account for the sampling method used and any non-response in survey responses. However, for this example, the classical Horvitz-Thompson estimator shall be considered.

Recall from Section 2.1, that hard calibration constraints can be written in the form $X'W = T$ or equivalently $A'G = T$, with $a_{ij} = d_i x_{ij}$. There is only one auxiliary variable in this example, thus $X$ and $A$ reduce to $12 \times 1$ vectors. The size of the 12 sampled cities in 1920 is given in the $12 \times 1$ vector $X$, where $X = (93, 77, 61, 87, 116, 2, 30, 172, 36, 64, 66, 60)'$. The size of the 12 sampled cities in 1930 is known, and given in the $12 \times 1$ vector $Y$, where $Y = (104, 89, 69, 105, 130, 50, 111, 183, 46, 77, 86, 57)'$.

Note that $X'D = A'\mathbf{1} = 3528 \neq 5054$. Also, the value of $Y'D$ is approximately 4520 which is much smaller than the known value of 6262. Therefore, for the initial weights $G = \mathbf{1}$, the constraint $A'G = T$ is not satisfied and our estimate does not approximate the true total of the $Y$-variable well. This motivates the need to calibrate.

Several approaches to calibrating the $g$-weights are considered, and the affect this has on the estimates $Y'W$ is explored. Figure 18 shows the $g$-weights obtained when optimizing (17) for the functions $\phi^{(1)}$, $\phi^{(2)}$ and $\phi^{(3)}$ using classical hard calibration, i.e. $L$ and $U$ are taken as vectors whose entries are $-\infty$ and $\infty$, respectively. The case $q_i = d_i$ is considered in (19). Figure 18(a) shows the calibrated weights when the constraint $\mathbf{1}'G = 12$ is not imposed. The calibrated weights obtained when this constraint is included in the optimization are shown in Figure 18(b).




(a) $g$-weights for functions $\phi^{(1)}$, $\phi^{(2)}$ and $\phi^{(3)}$ with the sum of weights unconstrained

(b) $g$-weights for functions $\phi^{(1)}$, $\phi^{(2)}$ and $\phi^{(3)}$ with the sum of weights constrained

Figure 18: Comparison of $g$-weights with 1 for the functions $\phi^{(1)}$ (red, cross), $\phi^{(2)}$ (blue, plus) and $\phi^{(3)}$ (green, circle).

For these functions, observe that not imposing the constraint $\mathbf{1}'G = 12$ results in all the weights increasing from, or remaining at, their initial value of 1. It can be verified that the calibrated weights for each of these functions satisfy the constraint $A'G = T$. In all cases, $\mathbf{1}'G > 12$ due to the calibrated weights being larger than the initial weights of 1, and all estimates of $Y'W$ are approximately 6840 (recall the true value is 6262). As all the weights have increased, our estimate $Y'W$ has over estimated the true value. However, it has improved on the original estimator of $Y'D = 4520$.

Imposing the extra constraint $\mathbf{1}'G = 12$ results in weights both above and below 1. One of the $g$-weights for function $\phi^{(1)}$ (indexed 6 in Figure 18(b)) is negative,

whilst the weight indexed 8 has taken a large value in comparison to the other $g$-weights. For functions $\phi^{(2)}$ and $\phi^{(3)}$, there is not a negative weight at index 6; however, the value of the weight at index 8 is still large in comparison with the other weights. Thus, whilst functions $\phi^{(2)}$ and $\phi^{(3)}$ prevent negative weights, they do not prevent large positive weights. For these weights, $A'G = 5054$, as expected. The estimate of $Y'W$ is approximately 5760. Compare this with the true value of 6262. In this case, the total size of the 49 cities has been underestimated by approximately 600,000.

Note that the behaviour of the weights for functions $\phi^{(4)}$ and $\phi^{(5)}$ is very similar to that for functions $\phi^{(2)}$ and $\phi^{(3)}$. Plots of the weights comparing functions $\phi^{(1)}$, $\phi^{(4)}$ and $\phi^{(5)}$ are very similar to the plots in Figs. 18(a) and 18(b). Hence weights for functions $\phi^{(4)}$ and $\phi^{(5)}$ shall not be plotted here. These functions are seldom used in practice, and struggle to prevent the weights taking large values since there is a lack of penalty for large positive values.

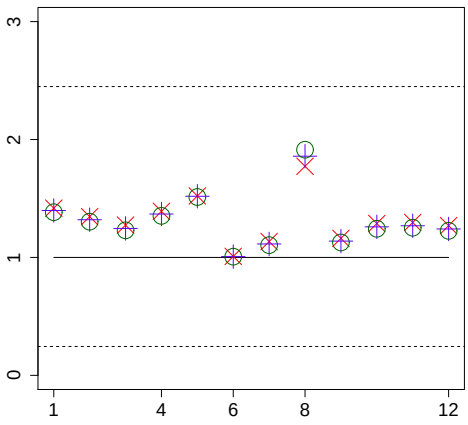
To overcome the issue of negative weights in the previous problem, one may simply consider projecting any weights falling outside of the bounds defined by $L$ and $U$ back onto the boundary values. Choosing $l = 12/49$ and $u = 120/49$ for the example above (so that the weights $d_i$ are restricted between 1 and 10) gives weights such that $A'G = 4822.967 \neq 5054 = T$. So by simply re-scaling our weights we no longer satisfy the hard calibration constraint. The estimate $Y'W$ is approximately 5520, meaning we are now underestimating the true value of 6262 by approximately $700,000$. This approach represents one step of an algorithm used by several of the calibration packages that are presented in Section 3.6. The algorithm continues solving and projecting weights until the hard calibration constraint $A'G = T$ is satisfied.

An alternative method for overcoming the issue of negative and extreme weights, is to include the constraint $L \leq G \leq U$ as part of the optimization procedure. Consider vectors $L$ and $U$ with repeated entries $l$ and $u$, respectively, where $0 \leq l < 1 < u \leq \infty$. Any feasible solution to this problem is guaranteed to be within the bounds pre-specified by the user. However, recall from Section 2.1 that the feasible solution of this problem may be empty depending on the choice of $L$ and $U$.

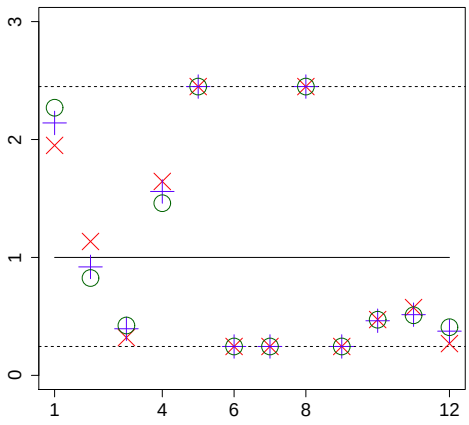
Returning to our example, suppose the we impose the $g$-weight bounds $L \leq G \leq U$ where $L = (l, l, ..., l)'$ and $U = (u, u, ..., u)'$ are both $12 \times 1$ vectors. Let $l = \frac{12}{49}$ and $u = \frac{120}{49}$ so each $g$-weight $g_i$ $(i = 1, \ldots, n)$ will be bounded between $\frac{12}{49}$ and $\frac{120}{49}$, whilst the weights $w_i$ will be bounded between 1 and 10.

Figure 19 shows the $g$-weights obtained by optimizing (17) for functions $\phi^{(1)}$, $\phi^{(2)}$ and $\phi^{(3)}$. Figure 19(a) shows the calibrated weights when we do not impose the constraint $\mathbf{1}'G = 12$. Figure 19(b) shows the calibrated weights when we include this constraint.

For the weights in Figure 19(a), observe that when we do not impose the constraint $\mathbf{1}'G = 12$, all the weights increase from, or remain at, their initial value of 1. The weights in Figure 19(a) are identical to those in Figure 18(a). However, in Figure 19(b), we see that imposing the extra constraint $\mathbf{1}'G = 12$ results in weights that are distributed both above and below 1. Many of the weights are near the upper and lower bounds $u$ and $l$, respectively. The weights in Figure 19(b) are different from those in Figure 18(b).




(a) $g$-weights for functions $\phi^{(1)}$, $\phi^{(2)}$ and $\phi^{(3)}$ with the sum of weights unconstrained



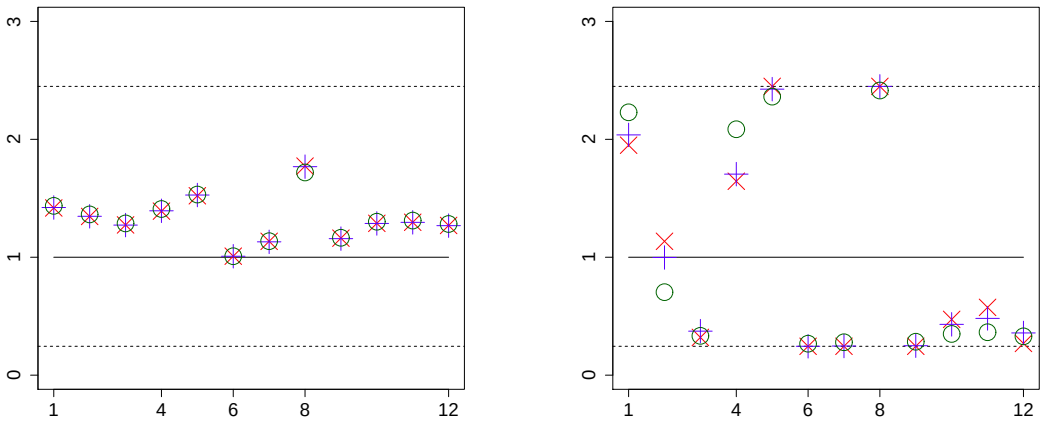

(b) $g$-weights for functions $\phi^{(1)}$ (red, cross), $\phi^{(2)}$ (plus) and $\phi^{(3)}$ (circle) with the sum of weights constrained

Figure 19: Comparison of $g$-weights with 1 for the functions $\phi^{(1)}$ (red, cross), $\phi^{(2)}$ (blue, plus) and $\phi^{(3)}$ (green, circle); dotted lines indicate bounds.

Note that the behaviour of the weights for functions $\phi^{(4)}$ and $\phi^{(5)}$ is very similar to that for functions $\phi^{(2)}$ and $\phi^{(3)}$, both with and without the constraint $\mathbf{1}'G = 12$ imposed. Hence, we do not plot the weights for these functions here.

Recall the relationship $w_i = d_i g_i$. Since the vector of initial weights $D$ is given, and we have calculated the $g$-weights, we can now compute the weights $w_i$. Computing the weights $w_i$ for function $\phi^{(1)}$ from the $g$-weights in Figure 19(b) gives the same weights as those derived in [29].

Figure 20 shows the $g$-weights obtained by optimizing (17) for the functions $\phi^{(1)}$, $\phi^{(6)}$ and $\phi^{(7)}$. Figure 20(a) shows the calibrated weights when we do not include the sum of weights constraint $\mathbf{1}'G = 12$. Figure 20(b) shows the calibrated weights when the constraint is included within the optimization. There are clear differences in the $g$-weights with indices 2 and 4 when we optimize using different calibration functions.



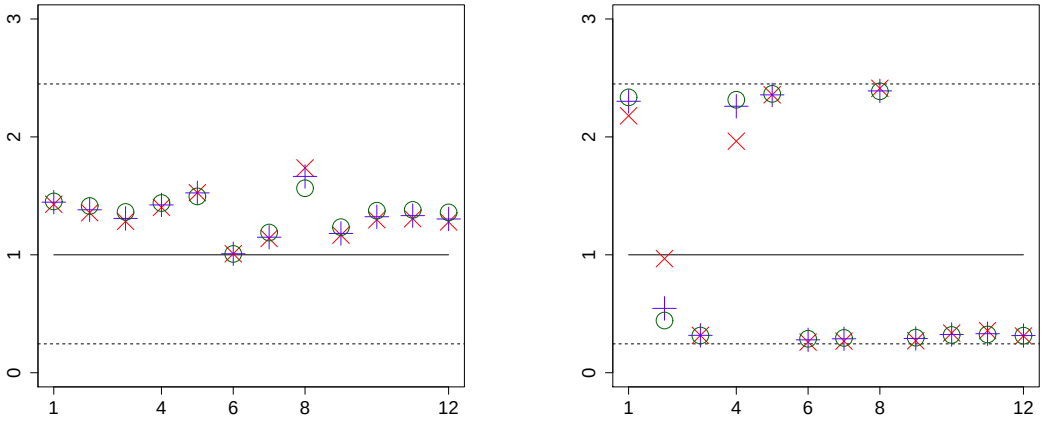

(a) $g$-weights for functions $\phi^{(1)}$, $\phi^{(6)}$ and $\phi^{(7)}$ with the sum of weights unconstrained

(b) $g$-weights for functions $\phi^{(1)}$, $\phi^{(6)}$ and $\phi^{(7)}$ with the sum of weights constrained

Figure 20: Comparison of $g$-weights with 1 for functions $\phi^{(1)}$ (red, cross), $\phi^{(6)}$ (blue, plus) and $\phi^{(7)}$ (green, circle); dotted lines indicate bounds.

Figure 21 shows the $g$-weights obtained by optimizing (17) for function $\phi^{(8)}$ with $\alpha$ chosen to be 0.2, 1 and 5. Figure 21(a) shows the calibrated weights when we do not impose the constraint $\mathbf{1}'G = 12$. Figure 21(b) shows the calibrated weights when we include this constraint within the optimization. Observe that as

the value of $\alpha$ increases, the algorithm tends to move the weights more towards the boundaries.




(a) $g$-weights for function $\phi^{(8)}$ with $\alpha = 0.2$ (cross), $\alpha = 1$ (plus) and $\alpha = 5$ (circle) with the sum of weights unconstrained

(b) $g$-weights for function $\phi^{(8)}$ with $\alpha = 0.2$ (cross), $\alpha = 1$ (plus) and $\alpha = 5$ (circle) with the sum of weights constrained

Figure 21: Comparison of $g$-weights with 1 for function $\phi^{(8)}$; dotted lines indicate bounds.

Again, we observe that when the constraint $\mathbf{1}'G = 12$ is not imposed, the weights all increase or remain at the initial values of 1. As our initial estimate of $Y'D$ is underestimating the true total of all the $y$-values from the population, the weights increase to give estimates $Y'W$ that are generally closer to the true value than the estimate $Y'D$.

When the constraint $1'G = 12$ is imposed, the weights are more evenly distributed above and below 1. More of the weights move towards the boundary values imposed by $L$ and $U$. Since we have added an additional constraint to the calibration, this increases the complexity of the calibration problem. In practice, it should be verified that this constraint has meaning and is necessary. In Chapter 5, soft calibration is considered for investigating how restrictive the constraint $\mathbf{1}'G = 12$ actually is.

In summary, not imposing the constraint $\mathbf{1}'G = 12$ results in calibrated weights that are less variable than the calibrated weights obtained when this constraint is included. For this example, we saw that when the constraint $\mathbf{1}'G = 12$ was

not included, the calibrated weights all increased from the initial values of 1 but did not exhibit any extremal behaviour, lying well within the $g$-weight bounds. However, including the constraint $\mathbf{1}'G = 12$ gave calibrated weights that were more variable and likely to move towards the boundaries.

This shows how the inclusion of additional calibration constraints can have an adverse and often undesirable effect on the final calibrated weights. In practice, care should be taken to ensure the variables and constraints included as part of the calibration are suitable for the problem at hand. However, in practice, this is often not the case. For example, estimates of unemployment are obtained every quarter using the same calibration variables and constraints from quarterly Labour Force Survey datasets (albeit with different values due to different samples). However, whilst some variables may be suitable in some quarters, they may have an adverse effect on the calibration weights and estimates in other quarters.

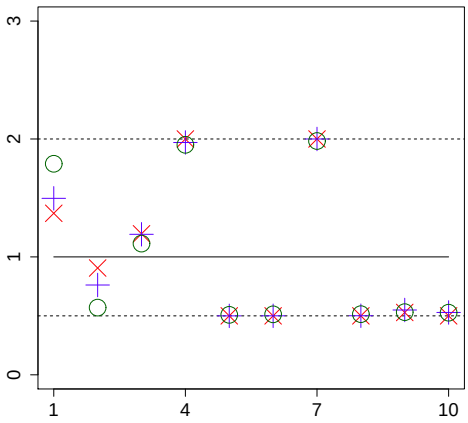
For the remaining examples in this chapter, we shall explore the effects the choice of $L$ and $U$ have on the calibrated weights $G$. In all the examples we will include the constraint $\mathbf{1}'G = n$ (where $n$ denotes the sample size), and take $q_i = d_i$ in (19).

### 4.3.2 Example 2: Changing the Upper and Lower Bounds

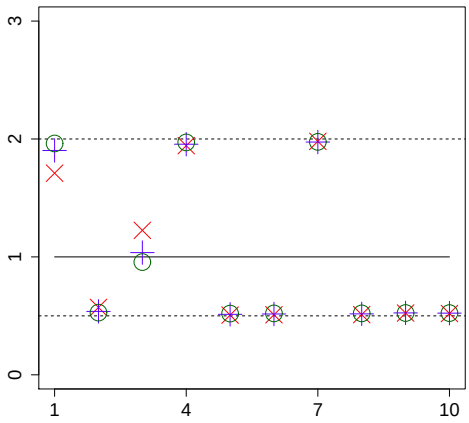
Suppose we are given the vector $X = (93, 77, 87, 116, 2, 30, 172, 36, 64, 60)'$ and the $10 \times 1$ vector of initial weights $D = (4, 4, ..., 4)'$. The parameter value $T = 3900$ is assumed known. Recall that we impose the upper and lower bounds $U = (u, u, ..., u)'$ and $L = (l, l, ..., l)'$, where $U$ and $L$ are both $10 \times 1$ vectors whose entries are $u$ and $l$, respectively. Consider the case $l = 1/u$. The objective is to find the smallest value of $u$ such that optimization problem (17) has a feasible solution. In this example, experimentation gave the smallest value of $u$ as approximately 2.0.

In Figure 22 we plot the calibrated weights when we take $l = 1/2$ and $u = 2$. In this case, solving the optimization problem (17) for functions $\phi^{(1)}$, $\phi^{(6)}$ and $\phi^{(7)}$

gives the weights in Figure 22(a). Figure 22(b) shows the weights for function $\phi^{(8)}$ with $\alpha = 0.2$, $\alpha = 1$ and $\alpha = 5$.




(a) Weights obtained for $\phi^{(1)}$ (red, cross), $\phi^{(6)}$ (blue, plus) and $\phi^{(7)}$ (green, circle)



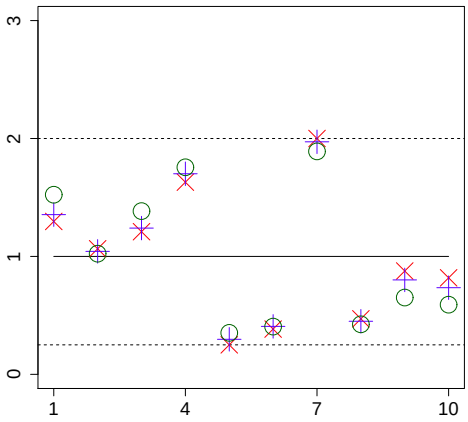

(b) Weights obtained for $\phi^{(8)}$ with $\alpha = 0.2$ (red, cross), $\alpha = 1$ (blue, plus) and $\alpha = 5$ (green, circle)

Figure 22: Comparison of weights for functions $\phi^{(1)}$, $\phi^{(6)}$, $\phi^{(7)}$, and $\phi^{(8)}$ for various $\alpha$ with $l = 1/2$ and $u = 2$; dotted lines indicate bounds.

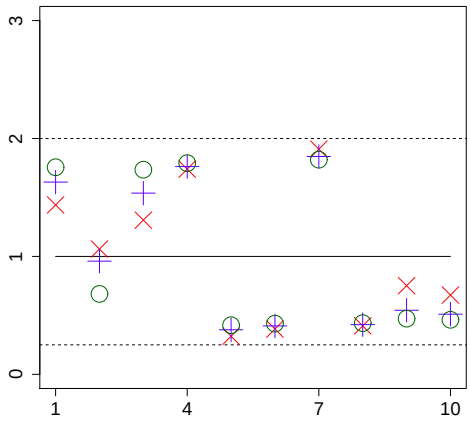
For this example, a feasible solution to problem (17) exists for the (approximate) bounds $0 \leq l \leq 1/2$ and $u \geq 2$. Let us consider the effect that changing the values of $l$ and $u$ has on the calibrated weights.

Figure 23 shows the calibrated weights when $l = 1/4$ and $u = 2$. In Figure 23(a) we plot the weights for functions $\phi^{(1)}$, $\phi^{(6)}$ and $\phi^{(7)}$ whilst in Figure 23(b) we plot the weights for function $\phi^{(8)}$ with $\alpha = 0.2$, $\alpha = 1$ and $\alpha = 5$. Reducing the lower bound results in fewer weights taking values at the lower bound. Note that the calibrated weights for function $\phi^{(8)}$ tend to move towards the boundaries more than the weights obtained for functions $\phi^{(1)}$, $\phi^{(6)}$ and $\phi^{(7)}$, with this tendency more evident as the value of $\alpha$ increases.

Now consider the effect of increasing $u$. In Figure 24, we keep $l = 1/4$ and consider the calibrated weights when $u = 4$. In Figure 24(a) we plot the calibrated weights for the functions $\phi^{(1)}$, $\phi^{(6)}$ and $\phi^{(7)}$ whilst in Figure 24(b) we plot the calibrated weights for function $\phi^{(8)}$ with $\alpha = 0.2$, $\alpha = 1$ and $\alpha = 5$. Increasing the upper



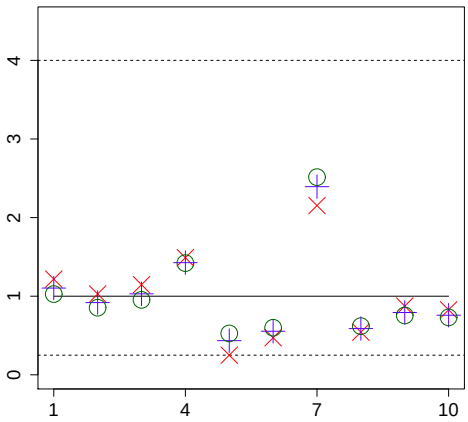

(a) Weights obtained for $\phi^{(1)}$ (red, cross), $\phi^{(6)}$ (blue, plus) and $\phi^{(7)}$ (green, circle)



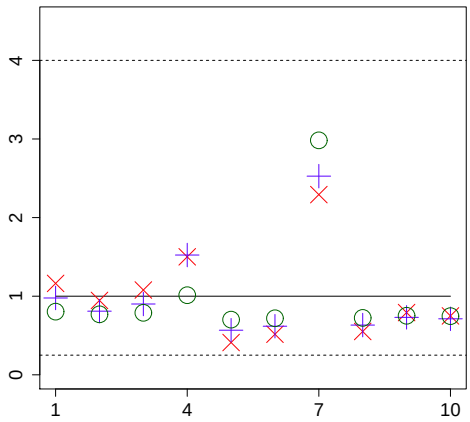

(b) Weights obtained for $\phi^{(8)}$ with $\alpha = 0.2$ (red, cross), $\alpha = 1$ (blue, plus) and $\alpha = 5$ (green, circle)

Figure 23: Comparison of weights for functions $\phi^{(1)}$, $\phi^{(6)}$, $\phi^{(7)}$, and $\phi^{(8)}$ for various $\alpha$ with $l = 1/4$ and $u = 2$ (dotted lines indicate bounds)

bound has resulted in some of the weights increasing slightly in comparison to the weights in Figure 23. However, there are no weights on the upper bound.




(a) Weights obtained for $\phi^{(1)}$ (red, cross), $\phi^{(6)}$ (blue, plus) and $\phi^{(7)}$ (green, circle)




(b) Weights obtained for $\phi^{(8)}$ with $\alpha = 0.2$ (red, cross), $\alpha = 1$ (blue, plus) and $\alpha = 5$ (green, circle)

Figure 24: Comparison of weights for functions $\phi^{(1)}$, $\phi^{(6)}$, $\phi^{(7)}$, and $\phi^{(8)}$ for various $\alpha$ with $l = 1/4$ and $u = 4$ (dotted lines indicate bounds)

To conclude, this example has shown that taking $l = 1/u$ and minimizing the value of $u$ such that the calibration problem (17) has a feasilbe solution often results in many of the weights taking values at the boundaries. Increasing the value of $u$ gives extra freedom to the optimization problem and, as a result, there are typically fewer weights at the boundaries.

In the remaining two examples, we only consider the smallest value of $u$ for which the optimization problem (17) has a feasible solution when $l = 1/u$. The phenomenon of weights clustering at the boundary is further explored. An investigation of whether certain calibration functions are more or less likely to give weights that approach the boundaries is also given.

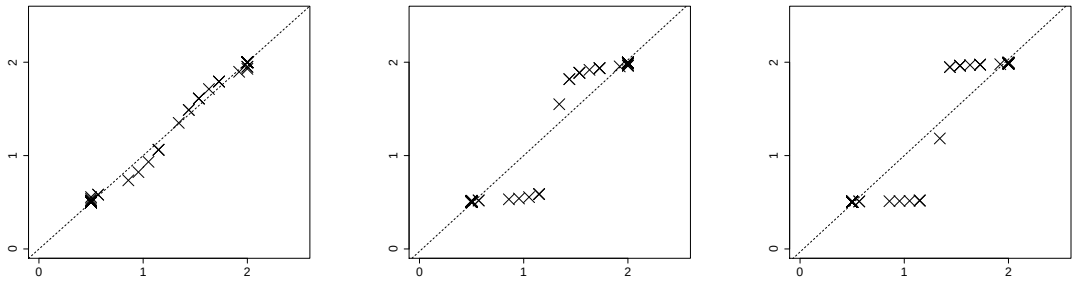
### 4.3.3 Example 3: Comparisons with the New Calibration Functions

Suppose we are given the $100 \times 1$ vector of initial weights $D = (5, ..., 5)'$ and suppose that $T = 49500$. The vector of auxiliary values $X$ is formed by extending the auxiliary vector from Example 4.3.2. Form a $100 \times 1$ vector that has the values from the auxiliary vector in Example 4.3.2 as its first ten entries. The remaining entries are formed by adding or subtracting constants to each of the first ten elements.

Impose the upper and lower bounds $U = (u, u, ..., u)'$ and $L = (l, l, ..., l)'$, where $L$ and $U$ are both $100 \times 1$ vectors whose entries are $u$ and $l = 1/u$, respectively. For this example, experimentation gives the smallest value of $u$ as approximately 2 (and so the largest corresponding value of $l$ is $\frac{1}{2}$).

In Figure 25, we compare the $g$-weights for functions $\phi^{(6)}$, $\phi^{(7)}$ and $\phi^{(8)}$ (taking $\alpha = 1$) with those for function $\phi^{(1)}$. In Figure 25(a), we observe that most of the points in the scatterplot lie on the main diagonal. This indicates the similarity of the weights for functions $\phi^{(1)}$ and $\phi^{(6)}$. However, in Figure 25(b), we observe that there are fewer weights on the diagonal. This indicates that, for function $\phi^{(7)}$, more of the weights approach the boundary. In Figure 25(c), we see this even more clearly with a distinct band of weights at the upper and lower bounds of

2 and $\frac{1}{2}$, respectively. This shows that functions $\phi^{(7)}$ and $\phi^{(8)}$ are more likely to send the $g$-weights towards the bounds.



(a) Comparison of weights for function $\phi^{(1)}$ against $\phi^{(6)}$

(b) Comparison of weights for function $\phi^{(1)}$ against $\phi^{(7)}$

(c) Comparison of weights for function $\phi^{(1)}$ against $\phi^{(8)}$ ($\alpha = 1$)

Figure 25: Comparison of weights for function $\phi^{(1)}$ against functions $\phi^{(6)}$, $\phi^{(7)}$ and $\phi^{(8)}$ ($\alpha = 1$), with $l = 1/2$ and $u = 2$

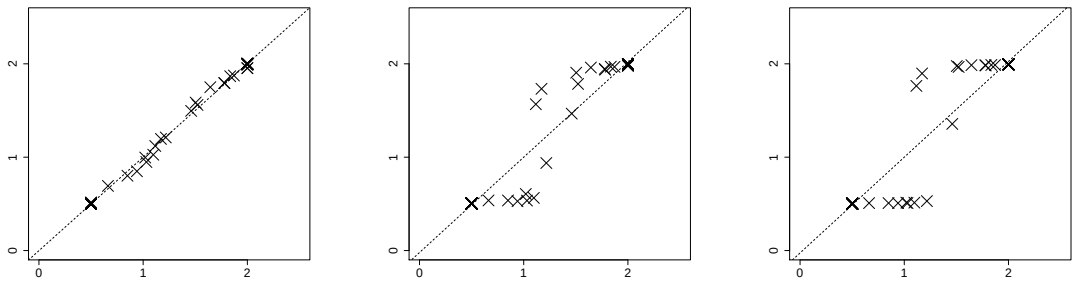
For the next example, we keep the sample size at $n = 100$ and increase the number of auxiliary variables to $m = 3$.

### 4.3.4 Example 4: Impact of Functions on CPU Times

Suppose we are given a $100 \times 1$ vector of initial weights $D = (5, ..., 5)'$, and know the vector of totals to be $T = (49500, 49540, 41000)'$. The $100 \times 3$ matrix of auxiliary values $X$ is defined as follows. The first column of $X$ is the same as the auxiliary vector from Example 3 in Section 4.3.3. For the second column of $X$ is chosen such that it does not highly correlate with the first column. For the third column, we take 100 values generated at random from a Normal distribution with mean 80 and standard deviation 48 (these are similar to the mean and standard deviations for the other columns).

Impose the lower and upper bounds $L = (l, l, ..., l)'$ and $U = (u, u, ..., u)'$, where $L$ and $U$ are both $100 \times 1$ vectors whose entries are $u$ and $l = 1/u$, respectively. For this example, experimentation gives the smallest value of $u$ as approximately $u = 2$ (and so the corresponding largest value of $l$ is $\frac{1}{2}$).

In Figure 26, we compare the calibrated weights using function $\phi^{(1)}$ with the calibrated weights for functions $\phi^{(6)}$, $\phi^{(7)}$ and $\phi^{(8)}$ ($\alpha = 1$).



(a) Comparison of weights for function $\phi^{(1)}$ against $\phi^{(6)}$

(b) Comparison of weights for function $\phi^{(1)}$ against $\phi^{(7)}$

(c) Comparison of weights for function $\phi^{(1)}$ against $\phi^{(8)}$ with $\alpha = 1$

Figure 26: Comparison of weights for the function $\phi^{(1)}$ against $\phi^{(6)}$, $\phi^{(7)}$ and $\phi^{(8)}$ ($\alpha = 1$)

Figure 26 has many similarities with Figure 25 in Example 4.3.3. Observe that the weights for functions $\phi^{(1)}$ and $\phi^{(6)}$ are very similar. However, the calibrated weights for functions $\phi^{(7)}$ and $\phi^{(8)}$ show clear differences to the calibrated weights for function $\phi^{(1)}$. Again, we observe the distinct band of weights at the upper and lower bounds of 2 and $\frac{1}{2}$ for functions $\phi^{(7)}$ and $\phi^{(8)}$, compared with the weights for functions $\phi^{(1)}$ and $\phi^{(6)}$ that are more evenly distributed between the upper and lower bounds.

Now the CPU times taken to obtain the weights in Figure 26 are compared. These CPU times were computed on a computer with an Intel(R) Core(TM) i7-4500U CPU Processor with 8GB of RAM. The CPU times are given in Table 12. Observe that the CPU times for functions $\phi^{(7)}$ and $\phi^{(8)}$ ($\alpha = 0.2$) are less than those for the classical functions $\phi^{(1)}$ and $\phi^{(6)}$. CPU time is related to the complexity of the optimization problem, see [43] on a comprehensive discussion of how to measure numerical complexity of an optimization problem.

The longest CPU time recorded was for function $\phi^{(6)}$. This is likely due to the slow convergence of the algorithm, as we have seen in the previous examples. Recall also that the algorithm for $\phi^{(1)}$ requires the weights that fall outside the bounds to be projected back to the bounds before the calibration problem is performed

again. This is likely to have resulted in the higher CPU time for this function in comparison to functions $\phi^{(7)}$ and $\phi^{(8)}$.

| Function | CPU Time (seconds) |
|---|---|
| $\phi^{(1)}$ | 0.609 |
| $\phi^{(6)}$ | 0.734 |
| $\phi^{(7)}$ | 0.544 |
| $\phi^{(8)}$ $(\alpha = 0.2)$ | 0.569 |
| $\phi^{(8)}$ $(\alpha = 1)$ | 0.559 |

Table 12: CPU times for various functions $\phi$ in solving the optimization problem (17) in Example 4

## 4.4 Summary

In this chapter, the choice of the objective function in the calibration problem has been explored. The influence of the function $\phi$, the main component of objective function, on the complexity of the optimization problem and the final solution has been studied. Two new calibration functions $\phi^{(7)}$ and $\phi^{(8)}$ have been suggested. These are more flexible than existing calibration functions in that they automatically take into account the constraint $L \leq G \leq U$. This could be of high importance in practice as the dimension of the problem (which is the size of the sample) may be very large.

In the case of large samples, there may not be a solution to the hard calibration problem defined by (19) and (17). In this case, it may be preferable to use soft calibration, either as a method for deriving calibrated weights or for assessing which of the constraints are performing poorly. In doing so a potentially difficult constrained optimization problem (17) has been replaced with a much simpler problem (18), which is an unconstrained convex optimization problem. The soft calibration problem shall be described further in the next chapter.

# 5 Soft Calibration

In this chapter, the soft calibration problem shall be presented. The previous chapters have focused on the hard calibration problem. Whilst the hard calibration is more frequently used in practice, it is not guaranteed to have a solution. This is particularly prevalent in the case of strict upper and lower bounds for the $g$-weights.

One approach to resolve this problem is simply relaxing the bounds on the calibrated weights until a solution can be found. However, this can result in different bounds being used for different samples of the same survey. For example, the Labour Force Survey is conducted quarterly by the Office for National Statistics. Each quarterly sample is calibrated to Census data. Whilst a particular choice of lower and upper bounds may be suitable for the data from one quarter, these bounds are not guaranteed to work for the next quarter.

Another approach is to use soft calibration. Instead of relaxing the bounds on the calibration weights, the calibration constraints are relaxed. There is a practical benefit to this, since the totals used to form the calibration constraints are often themselves estimated from Census data. Whilst these totals are often taken to be the 'truth', they will inevitably have their own margin of error. Therefore, a small relaxation of the calibration constraints can help account for the error in the calibration totals.

There are two uses of soft calibration considered in this chapter. Firstly, the soft calibration problem shall be presented as a calibration method in its own right. Despite the benefits described above, soft calibration is not deemed a viable method by many practitioners. However, the second use of soft calibration is for identifying 'problematic' constraints in the hard calibration problem. This has practical appeal as a diagnostic tool before running the hard calibration problem.

## 5.1 Introduction

Recall that the soft calibration problem considered in this thesis is

$$\Phi(G) + \Psi(A'G, T) \to \min_{G \in \mathbb{G}}, \text{ where } \mathbb{G} = \{G : L \leq G \leq U\}. \tag{23}$$

where

$$\Phi(G) = \Phi(g_1, \ldots, g_n) = \sum_{i=1}^{n} q_i \phi_i(g_i)\,. \tag{24}$$

Here $\phi$ is a specified calibration function and $q_1, \ldots, q_n$ are given non-negative numbers. In the majority of applications $q_i = d_i$ for all $i$; it is assumed that $q_i = d_i$ throughout this chapter. The vectors $L$ and $U$ are $n$-vectors of lower and upper bounds for the $g$-weights $G$, respectively, $A$ is a known matrix derived from the sample observations, and $T$ is an $m$-vector of known population totals.

The function $\Psi$ assesses the deviation between the population totals and the calibration estimator $A'G$. The functions $\Phi$ and $\Psi$ can take many forms, including any of the functions given in Chapter 4. However, the purpose of this chapter is to highlight the use of the calibration problem rather than explore the choice of the functions. Therefore, for simplicity, $\Phi$ and $\Psi$ shall only be considered to be quadratic functions. Soft calibration with other choices of functions remains an interesting area for further research.

Rewriting the soft calibration problem (23) using quadratic functions for $\Phi$ and $\Psi$ leads to the following optimization problem:

$$\sum_{i=1}^{n} q_i (g_i - 1)^2 + \beta^{-1}(A'G - T)'C(A'G - T) \to \min_{G \in \mathbb{G}}, \tag{25}$$

where $\mathbb{G} = \{G : L \leq G \leq U\}$, $q_1, ..., q_n$ are given non-negative numbers, $C$ is a user-specified $m \times m$ positive definite (usually diagonal) matrix and $\beta > 0$ is some constant.

In the objective function above, the first term above assesses the deviation between the calibrated weights and 1, whilst the second penalty controls the deviation between the calibrated estimates and the known population totals. The amount of

importance given to this penalty will determine how much the calibration constraints are relaxed. This is controlled by the value of the parameter $\beta$. The larger the value of $\beta$, the smaller the value of $\beta^{-1}$ and the less importance given to this term. However, for small values of $\beta$, $\beta^{-1}$ will be large and therefore greater importance is given to this term. Note that the function $\Psi$ considered in this chapter has the following form:

$$\Psi(A'G, T) = \beta^{-1}(A'G - T)'C(A'G - T) \tag{26}$$

Soft calibration is synonymous with ridge regression. The parameter $\beta$ here emulates a ridge parameter. Informally, the ridge parameter helps enable a solution to be found to the regression problem in cases when a solution otherwise could not be found. Similarly, the parameter $\beta$ can be used in soft calibration to enable solutions to be found when the corresponding hard calibration problem cannot be solved. Throughout this chapter, $\beta$ shall be referred to as the soft calibration paramter.

The classical approach to soft calibration is to minimize the objective function given in (25) without any restrictions imposed on the weights, i.e. the weight bounds $L \leq G \leq U$ are not included within the optimization. This method shall be referred to as classical soft calibration (see for example [8]). The value of the parameter $\beta$ is then varied so that the weights are within the upper and lower bounds. There are several problems with this method, that shall be described throughout this chapter.

However, formulating soft calibration via the optimization problem above allows the constraint $L \leq G \leq U$ to be included within the optimization algorithm and means the problem (23) can be solved directly. This is something that has not been considered or addressed in existing literature. For this approach, the choice of the parameter $\beta$ is determined in advance. This enables the same value of $\beta$ to be used for different sample datasets. Using the classical soft calibration approach, different $\beta$ values are often needed to ensure the weights fall within the specified bounds.

In Section 5.2, the classical soft calibration problem is considered. The drawbacks of this approach shall be discussed. Section 5.3 introduces the new approach to soft calibration, which considers soft calibration as a direct optimization method. The benefits of this approach shall be described and contrasted with classical soft calibration. Finally, Section 5.4 describes how soft calibration can be used as a diagnostic tool for identifying problematic calibration constraints.

## 5.2 The Classical Approach to Soft Calibration

The classical soft calibration problem was proposed both to deal with cases when the hard calibration problem has no solutions, and as a way to deal with negative and extreme weights. Classical soft calibration allows an analytic solution to be found to the optimization problem (25). Let $\mathbb{D}$ be an $n \times n$ diagonal matrix, whose entries are the weights $d_1, d_2, ...d_n$. Furthermore, take $q_i = d_i$ and let $\beta$ denote the soft calibration parameter. Then, for the classical soft calibration approach, the analytic form of the weights that satisfy optimization problem (25) is given by

$$G = \mathbf{1} + A\left(A'\mathbb{D}^{-1}A + \beta C^{-1}\right)^{-1}(T - A'\mathbf{1}). \tag{27}$$

This is an equivalent formulation of equation (2.4) from [8], expressed in terms of $g$-weights. The term $(A'\mathbb{D}^{-1}A + \beta C^{-1})^{-1}$ is similar to the inverse matrix term in ridge regression (see for example [50]).

Observe that this problem has not imposed any constraints on the calibrated weights. Whilst this method guarantees that a solution can be found to the calibration problem, it does not prevent weights becoming negative or extreme. Therefore, just as in the case of the quadratic function with no constraints in hard calibration, the solution may have negative and/or extreme weights.

However, to address this point, authors such as Beaumont and Bocci in [8] consider the effect of changing the parameter $\beta$ in (25). As $\beta$ tends to zero, the optimization problem (25) reduces to minimising the expression $(A'G - T)'C(A'G - T)$ for $G \in \mathbb{G}$. As this term is quadratic, the minimum occurs when $A'G - T = 0$ or equivalently $A'G = T$. This is the hard calibration constraint. Therefore, the case

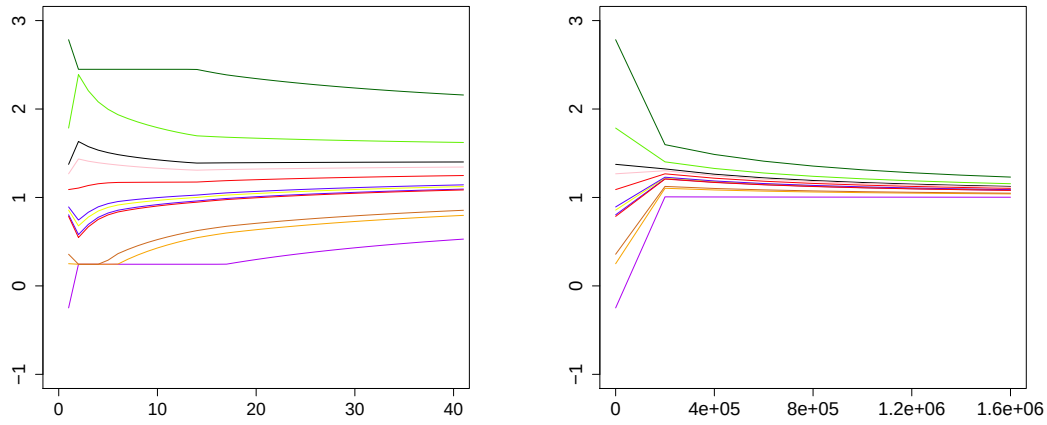
$\beta \to 0$ corresponds to solving the hard calibration problem (3). This is consistent with (27), since $\beta^{-1} \to \infty$ as $\beta \to 0$, which gives the expression for the $g$-weights in classical hard calibration using function $\phi^{(1)}$.

As $\beta$ tends to infinity, the term $(A'G - T)'C(A'G - T)$ becomes negligible. This results in the optimization problem (25) reducing to the problem of minimizing $\Phi(G) = \sum_{i=1}^{n} q_i \phi^{(1)}(g_i)$ for $G \in \mathbb{G}$, which is minimized at $G = \mathbf{1}$ (by definition of the function $\Phi$). Again, this is consistent with (27), since $\beta^{-1} \to 0$ as $\beta \to \infty$, and hence $A\left(A'\mathbb{D}^{-1}A + \beta C^{-1}\right)^{-1}(T - A'\mathbf{1})$ tends to zero giving $G = \mathbf{1}$.

Ideally, the value of the soft calibration parameter should be small. The value of $\beta^{-1}$ can be thought of as the relative importance of the term (26). The larger the value of $\beta^{-1}$, the more importance is placed on satisfying the calibration constraints. In contrast, the smaller the value of $\beta^{-1}$, the less importance is placed on satisfying the calibration constraints. Approximately satisfying the calibration constraints is very important, since one of the main motivating factors for calibration is consistency with known totals.

To illustrate the soft calibration problem, the example from Section 4.3.1 shall be revisited. Recall that the size of 12 cities in 1930 is known and the aim is to estimate the population total from 49 cities. The size of the 12 cities is known in 1920, as is the population total of the 49 cities from 1920. Using the standard notation, $T = 5054$ is the population total of the 49 cities in 1920 (in thousands), $D = (49/12, ..., 49/12)'$ are the initial weights and the size of each of the 12 sampled cities in 1930 is given in $X = (93, 77, 61, 87, 116, 2, 30, 172, 36, 64, 66, 60)'$ Recall that multiplying the entries in the $i$-th row of $X$ by the $i$th initial weight gives the entries of the matrix $A$.

In Figure 27, the weights given by (27) are plotted as the value of $\beta$ varies. The values of $\beta$ are plotted against the calibrated weights. For simplicity, take $C = I_m$, where $I_m$ denotes the $m \times m$ identity matrix. Figure 27(a) plots the weights for values of $\beta$ from 0 to 40. This plot confirms the earlier assertions that as $\beta \to 0$, $G$ tends to the classical hard calibration weights. Figure 27(b) plots the weights for values of $\beta$ between 0 and $1.6 \times 10^6$. This plot confirms that as $\beta \to \infty$, the $g$-weights tend to the initial values of 1.




(a) Soft calibration weights for $\beta$ from 0 and 40

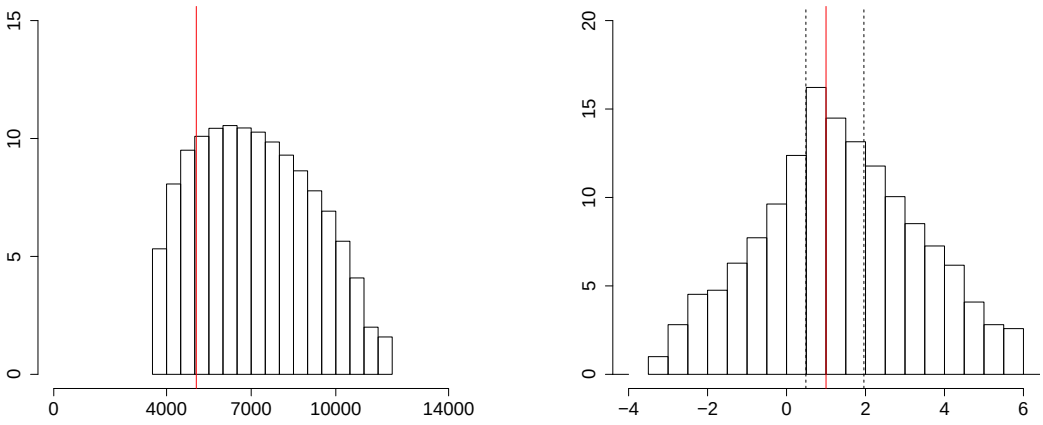
(b) Soft calibration weights for $\beta$ from 0 to $1.6 \times 10^6$

Figure 27: Plots of classical soft calibration weights (27) as a function of $\beta^{-1}$

When deriving the explicit solution, (27), to the classical soft calibration problem, there are no constraints specified on the weights $G$. However, suppose that the weight constraint $L \leq G \leq U$ is required. Observe from Figure 27(a) that as the value of $\beta$ increases (and so $\beta^{-1}$ decreases), the range of the weights decreases. In classical soft calibration, having obtained the analytic solution (27) for the calibrated weights, the approach to satisfying the constraint $L \leq G \leq U$ is to choose the smallest value of $\beta$ for which the weights in (27) are within the specified bounds. Clearly, the value of $\beta$ that satisfies the constraints $L \leq G \leq U$ is sample dependent.

Returning to Example 1 from Section 4.3.1, suppose the lower and upper bounds of $l = 12/49$ and $u = 120/49$ are required. These bounds could be satisfied using the hard calibration problem. In order to satisfy these bounds for classical soft calibration, the smallest value of $\beta$ that gives weights within the required bounds is approximately 9.0. This is a relatively large value of $\beta$, since $\beta^{-1} = 1/9$, and there is relatively little importance on the term (26).

Note that in this case the values of the calibration constraints are $\mathbf{1}'G = 13.527 \neq 12$ and $A'G = 5053.899 \neq 5054$, therefore the constraints $\mathbf{1}'G = 12$ and $A'G = T$ are no longer satisfied. Having relaxed these constraints in the soft calibration penalty, there will inevitably be some variation between $A'G$ and $T$ and between




(a) $A'G$ for 10000 random samples of size 12, vertical line at 5054 ($A'G = 5054$ is hard constraint)

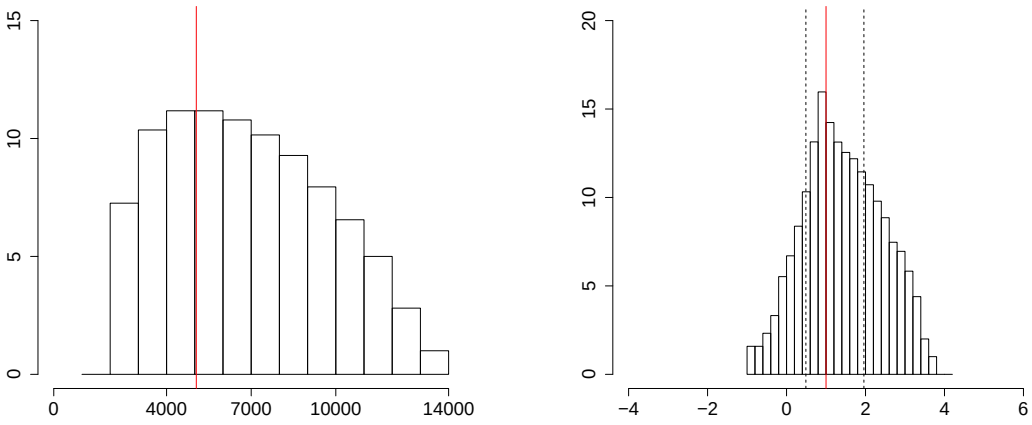
(b) $g$-weights for 10000 random samples of size 12, vertical line at 1 (initial weights), dashed lines indicate bounds

Figure 28: Plots of $A'G$ and $g$-weights that satisfy optimization problem (27) for $\beta = 0.1$

$\mathbf{1}'G$ and 12. The larger the value of $\beta$, the smaller the value of $\beta^{-1}$ and less importance is assigned to the penalty (26). However, for large values of $\beta$ there is less variation in the weights. In contrast, for small values of $\beta$, the penalty (26) is given more importance allowing less variation between $A'G$ and $T$ and between $\mathbf{1}'G$ and 12. However, in this case there will be greater variability in the weights.

To illustrate this, 10,000 simple random samples of size 12 are taken from the data in [14] used for throughout this example. Figure 28 shows the distribution of weights and values of $A'G$ with $\beta = 0.1$. Figure 29 shows the distribution of weights and values of $A'G$ for $\beta = 9$, as required for this example to ensure the weights are between $L$ and $U$. Observe that although $\beta = 9$ gave $g$-weights satisfying the bounds $L \leq G \leq U$ for one sample, this value of $\beta$ does not guarantee that the $g$-weights will satisfy these bounds for every sample.

Interesting comparisons can be drawn between the histograms in Figure 28 and Figure 29. The distribution of the estimates $A'G$ is much less variable in Figure 28, since the small value of $\beta$ has assigned relatively high importance to the term (26). However, the distribution of weights is more variable in Figure 28, since




(a) $A'G$ for 10000 random samples of size 12, vertical line at 5054 ($A'G = 5054$ is hard constraint)

(b) $g$-weights for 10000 random samples of size 12, vertical line at 1 (initial weights), dashed lines indicate bounds

Figure 29: Plots of $A'G$ and $g$-weights that satisfy optimization problem (27) for $\beta = 9$

the weights are forced to deviate more in order to satisfy the more stringent constraints.

Another important conclusion from these histograms is that the soft calibration parameter $\beta$ will vary considerably from sample to sample in order to satisfy imposed weight constraints. Many of the weights in Figures 28(b) and 29(b) lie well beyond the weight constraints indicated by the vertical dashed lines. Whilst the parameter $\beta = 9$ gave weights that satisfied the bounds for the sample considered previously, it clearly will not work for every sample.

This is the main drawback of classical soft calibration. The parameter $\beta$ is decided as an 'after-thought' of the process, but arguably this should be decided up front. The changing of the value of the $\beta$ is purely an after 'trick' to satisfy the required weight bounds.

In the next section, a new approach to soft calibration shall be proposed that uses direct optimization. The soft calibration problem was framed in Chapter 2. Since soft calibration can be framed as an optimization problem, direct optimization methods can be used to solve the problem. There are two clear advantages of this

method over classical soft calibration. Firstly, the weight constraints can be incorporated as part of the problem. Secondly, the ridge parameter $\beta$ is determined up front, and a solution to the problem can always be found independent of the value of $\beta$.

## 5.3 A New Approach to Soft Calibration

In the previous section, the classical soft calibration problem was described. Two main problems were identified. Firstly, the value of $\beta$ is determined after the calibration has been performed, in order to adjust the weights until they fall within pre-determined bounds. Secondly, the value of $\beta$ needed to satisfy these bounds is entirely sample dependent.

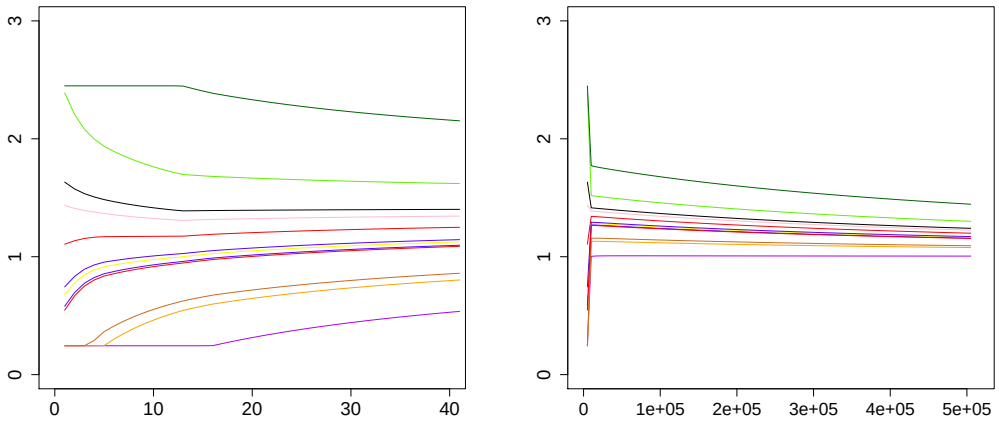
It is unclear why this is still the only main methodology that exists in the area of soft calibration. Of course, there is the practical appeal of being able to derive the general solution given in (27). However, software packages and algorithms are now so advanced that the need to derive an explicit formula for the general solution seems unnecessary.

Instead of this classical approach, soft calibration can be considered as the optimization problem described in (23). As stated in Section 2.1, optimization problem (23) has a solution for any value of $\beta > 0$. Therefore, given any $L$ and $U$, a solution to optimization problem (23) can always be found, independent of the choice of $\beta$. That is the key factor in making this approach different to classical soft calibration.

Returning to the example considered in the previous section, which considered classical soft calibration for the example from Section 4.3.1, the same data set is calibrated using the optimization problem (23) with $L \leq G \leq U$ where $L = (l, ..., l)'$ and $U = (u, ..., u)'$ are $12 \times 1$ vectors with entries $l = \frac{12}{49}$ and $u = \frac{120}{49}$, respectively. Recall that small values of $\beta$ give a solution that is close to the hard calibration solution, and ensure that the calibration constraints are approximately satisfied. Taking $\gamma = 0.01$, soft calibration weights can be obtained that are very similar to those derived for hard calibration in Section 4.3.1.

In this instance, solving problem (23) has little advantage over solving the corresponding hard calibration problem (3). This is an important point, since in cases when the hard calibration problem can be solved, there will be little or no difference between the solutions derived from both methods.

Solutions to the optimization problem (23) are derived for various values of the soft calibration parameter $\beta$. The resulting weights are shown in Figure 30. Once again, for small values of $\beta$ the solution tends to the hard calibration weights, whilst for large values of $\beta$ the weights tend to 1.




(a) Soft calibration weights for $\beta$ from 0 and 40

(b) Soft calibration weights for $\beta$ from 0 and $5 \times 10^5$

Figure 30: Plots of weights that satisfy the optimization problem (27) as a function of $\beta$

However, hard calibration will have a 'breaking' point, that is to say that once the upper and lower bounds are too tight it will not be possible to find a solution to the problem. However, soft calibration will still be able to find an approximate solution in this case. Furthermore, as shall be described in Section 5.4, the soft calibration can also help understand why a solution cannot be found to the corresponding hard calibration problem.

Returning to the example, consider the bounds $l = 24/49$ and $u = 96/49$, corresponding to bounding the weights $w_i$ between the lower and upper bounds of 2 and 8, respectively. In this case, there is no feasible solution to the hard calibration problem. Solving this problem using classical soft calibration requires a

value of $\beta = 16$ to ensure that the weights are between the specified bounds. In this case $\beta^{-1} = 1/16$, which indicates that the calibration constraints are given very little importance due to the 'restrictive' weight bounds.

Now consider using the new direct optimization approach for soft calibration. Again imposing the lower and upper bounds of $l = 24/49$ and $u = 96/49$, respectively, and taking $\beta = 10^{-9}$, the calibrated weights $G$ are such that the constraint values are $A'G = 5053.910$ and $\mathbf{1}'G = 13.435$. The hard calibration constraints require $A'G = 5054$ and $\mathbf{1}'G = 12$. The constraint $A'G = 5054$ is virtually satisfied, however the constraint $\mathbf{1}'G = 12$ is not fully met. This suggests that the condition $\mathbf{1}'G = 12$ was too restrictive, and this will be further discussed in the next section.

The important point here is that the value of $\beta$ was determined in advanced, and not decided based on the sample. Furthermore, a solution was found directly that was able to satisfy the given weight bounds.

This is a very elementary introduction to a method that guarantees a solution to the calibration problem. The key contribution in this thesis is the methodology and framing of soft calibration as an optimization problem. Much more investigation is needed to fully highlight the benefits of this approach. Furthermore, alternative soft calibration functions $\Phi$ and $\Psi$ in (23) should be investigated.

Soft calibration has many practical benefits. A solution can always be found, no matter how strict the weight bounds or the calibration constraints. Additionally, the penalty for not satisfying the calibration constraints can be determined upfront (through the soft calibration parameter $\beta$). This is in contrast to classical soft calibration which guarantees a solution, but makes use of the soft calibration parameter to satisfy the weight bounds.

In the next section, the use of soft calibration as a diagnostic tool shall be explored. Whilst practitioners may not wish to adopt soft calibration as a direct calibration tool, it has the benefit of being able to identify problematic constraints and give a clear indication of whether a solution could be found to the corresponding hard calibration problem.

## 5.4 Soft Calibration as a Diagnostic Tool

In this section, the new approach to soft calibration as described in Section 5.3 shall be used as a tool for identifying problematic constraints and as a diagnostic tool that can be used before carrying out hard calibration.

Statistical offices are unlikely to adopt soft calibration as a methodology. The main argument for this is that hard calibration guarantees consistency, whilst soft calibration does not. However, a counter-argument to this statement would be that soft calibration guarantees a solution whilst hard calibration does not. Despite this, soft calibration could also be used as a diagnostic tool to investigate whether the corresponding hard calibration problem will have a solution.

Returning again to the example considered the previous two sections. When the lower and upper bounds were $l = \frac{12}{49}$ and $u = \frac{120}{49}$, the solution obtained via the new soft calibration method with $\gamma = 10^{-9}$ was virtually identical to the solution from hard calibration. This was in fact the case for all values of $\gamma$ less than 1. Furthermore, the calibration constraints were approximately satisfied, with differences between the sample estimates and the population totals of the order $1 \times 10^{-2}$ or less.

However, when the lower and upper bounds of $l = 24/49$ and $u = 96/49$ were used with $\gamma = 10^{-9}$, the calibrated weights $G$ were such that $A'G = 5053.910$ and $\mathbf{1}'G = 13.435$. Given the hard calibration constraints were $A'G = 5054$ and $\mathbf{1}'G = 12$, the constraint $A'G = 5054$ has been virtually satisfied. However, the constraint $\mathbf{1}'G = 12$ has not been satisfied. The value of the estimate is approximately 12% larger than the constraint value. This suggests that the condition $\mathbf{1}'G = 12$ was too restrictive.

This example demonstrates a clear application for soft calibration as a diagnostic tool. By running soft calibration first, the proximity of the estimates and the known constraint values can be examined to determine whether the hard calibration problem will have a solution. If the estimates and constraint values are virtually the same, this suggests that hard calibration will find a solution to the

problem. However, if the constraints are not satisfied approximately, there is unlikely to be a solution to the corresponding hard calibration problem.

In the case that the constraints are not met exactly, the user can then decide how to proceed. Of course, the weights obtained from the soft calibration problem could be used. Alternatively, an investigation of the sample data and the constraint values may be needed to identify any outliers and problematic values. Alternatively, the weight bounds can be relaxed slightly and the soft calibration performed again to diagnose the likelihood of a hard calibration solution.

## 5.5 Summary

In this section, the soft calibration problem has been introduced. Its use as a method for solving the calibration problem has been described, and shown to give virtually identical solutions to hard calibration in the cases of "well-behaved" constraints. Unlike hard calibration, soft calibration is guaranteed to give a solution to the calibration problem.

(recall that all constraints in (18) are taken into account due to a clever choice of the functions $\phi_i$). If $\beta$ is large then the solution of this problem is guaranteed to be very close to the solution of the original problem (17).

The use of soft calibration as a diagnostic tool has also been explored. This allows identification of challenging constraints that may lead to lack of convergence when applying the hard calibration problem.

In the next chapter, a new approach to calibration is proposed. This approach involves minimization of the mean squared error of the calibration estimator. This approach is practically appealing, since it is the variance and bias of the calibration estimators that are often of more interest to practitioners.

# 6 Mean Square Error Calibration

In the previous chapters, calibration has been presented as a technique for adjusting the sample weights assigned to sample members within a survey. Properties of these weights and corresponding estimates have been described, along with an investigation of how these weights change for various choices of calibration algorithms and functions.

Problems considered so far include negative weights, extreme weights and a lack of solution to the calibration problem. These have been addressed in several ways, including alternative calibration functions and algorithms and the use of soft calibration.

Despite this, it is often the variance and bias of the calibration estimates that are of more interest to practitioners than the weights themselves. Therefore, in this chapter, a new approach to calibration is proposed that adjusts the sample weights through direct minimization of the mean squared error (MSE) of the calibration estimator.

For this section, it is easier to derive the results using the calibration weights themselves instead of the $g$-weights. Therefore, we adapt the notation seen previously in terms of the calibrated weights $W$ rather than the $g$-weights $G$.

## 6.1 Introduction

Recall that the size of the population is denoted by $N$ and the size of the sample is denoted by $n$. Let $\pi_k$ denote the inclusion probability for the $k$-th member of the population ($k = 1, \ldots, N$). Let $\pi_{kl}$ denote the joint-inclusion probability for the $k$-th and $l$-th population units. The use of the word probability here may be misleading, in the sense that $\pi_k$ is not a probability itself, but rather a sum of probabilities for all of the samples that element $k$ appears in. Therefore, $\sum_{k=1}^{N} \pi_k = n$, and not 1. Furthermore, $\pi_{kl}$ denotes the sum of the probabilities for all samples that elements $k$ and $l$ appear in together.

The indices $1, \ldots, n$ shall be used to denote the sample members. Note that these do not, necessarily, correspond with the indices $1, \ldots, n, \ldots, N$ used for the population members.

A vector of initial sample weights $D = (d_1, \ldots, d_n)'$ is given. Assume that $d_i = \frac{1}{\pi_i}$, $i = 1, \ldots, n$. Since the inclusion probabilities, $\pi_i$, are always finite and positive, the initial weights $d_i$ will also be positive, that is: $d_i > 0$ for all $i$. As in the earlier chapters, it shall be assumed that the initial weights are known in advance and have been adjusted to account for biases and non-response in the sample.

Let $Y$ denote the variable of interest. For this variable, only the sample values are known. The unknown population total, mean or proportion needs to be estimated. This chapter focuses on the estimation of population totals.

To estimate the unknown population total, the estimator $Y'W = \sum_{i=1}^{n} w_i y_i$, where $w_i$ denotes the calibrated weight for the $i$-th sample member ($i = 1, \ldots, n$), $W = (w_1, \ldots, w_n)'$ and $Y = (y_1, \ldots, y_n)'$. This is a linear weighted estimator of the unknown population total. This unknown population total shall be denoted $T_Y$. The initial weights could be used, however calibrated weights are generally favourable since they usually give estimators with smaller variance.

In the process of calibrating the weights, known auxiliary information for $m$ variables is used. Let $X = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_n \end{pmatrix} = (x_{ij})_{i,j=1}^{n,m}$. The $(i,j)$-th entry $x_{ij}$ of $X$ denotes the value that the $i$-th member of the sample takes on the $j$-th auxiliary variable, where $i = 1, \ldots, n$ and $j = 1, \ldots, m$.

The population totals for the $m$ auxiliary variables are given in the vector $T_X = (t_1, \ldots, t_m)'$. Exact (hard) constraints can be written as $X'W = T_X$. These constraints are used for calibration of the weights. Soft constraints of the form $X'W \simeq T_X$ can also be used. Note the use of the subscript $X$ to distinguish the vector of known population totals $T_X$ for each of the $m$ auxiliary variables from the unknown population total $T_Y$ of the variable of interest, $Y$.

Additional constraints on $W$, in addition to $X'W = T_X$, can also be imposed. It is desirable for the calibrated weights to be non-negative; that is, $w_i \geq 0$ for all $i$ (see for example [3, 4, 23]). Recall the informal definition of a weight describing how many people in the population a sample member represents. Negative weights suggest that the sample member does not represent anyone. Clearly a sample member should represent themselves, and it is desirable that they represent a certain section of the population to have made the inclusion of this member in the sample worthwhile.

Stricter conditions on the calibrated weights $W$ are often imposed of the form $L \circ D \leq W \leq U \circ D$, where $L \circ D = (l_1 d_1, \ldots, l_n d_n)'$ and $U \circ D = (u_1 d_1, \ldots, u_n d_n)'$ are some given $n \times 1$ vectors, and $\circ$ denotes element wise multiplication. This is synonymous to the constraints $L \leq G \leq U$ that have been seen in the previous chapters.

If $l_i = 0$ and $u_i = \infty$ for all $i$, then the constraint $l_i d_i \leq w_i \leq u_i d_i$ coincides with the simple non-negativity constraint $w_i \geq 0$. In the majority of practical problems, $l_i = l$ and $u_i = u$ for all $i$ with $0 \leq l < 1 < u \leq \infty$, where strict inequalities $l > 0$ and $u < \infty$ are very common.

There are three common choices of the vectors $L = (l_1, \ldots, l_n)'$ and $U = (u_1, \ldots, u_n)'$, which have also been seen in previous chapters. These are:

(a) no constraints: $l_i = -\infty$ and $u_i = \infty$ for all $i$;

(b) non-negativity constraint: $l_i = 0$ and $u_i = \infty$ for all $i$;

(c) general constraints: $0 \leq l_i < 1 < u_i \leq \infty$.

The feasibility domain $\mathbb{W}$ for the vector of calibrated weights $W$ is defined to be

$$\mathbb{W} = \{W = (w_1, \ldots, w_n)' : \ L \circ D \leq W \leq U \circ D \text{ and } X'W = T_X\}, \qquad (28)$$

where $L, U, D \in \mathbb{R}^n$, $T_X \in \mathbb{R}^m$ and $X \in \mathbb{R}^{n \times m}$ are all given. Note that if the bounds $L \circ D \leq W \leq U \circ D$ for $W$ are too narrow, then the feasible domain $\mathbb{W}$ may be empty due to the strict requirement that $X'W = T_X$.

An alternative feasibility domain $\mathbb{W}_1$ for the vector of calibrated weights $W$ is defined to be

$$\mathbb{W}_1 = \{W = (w_1, \ldots, w_n)' : \ L \circ D \leq W \leq U \circ D \text{ and } X'W \simeq T_X\}, \qquad (29)$$

where $L, U, D \in \mathbb{R}^n$, $T_X \in \mathbb{R}^m$ and $X \in \mathbb{R}^{n \times m}$ are all given. Note that, in this case, the feasible domain is always non-empty. This corresponds to the constraints that have been seen for soft calibration in the previous chapter. Whilst the hard calibration with weight constraints is not guaranteed to have a solution, a solution can always be found in the corresponding soft calibration case.

For the development of this method, hard calibration constraints shall be the main focus. Practitioners typically prefer the use of hard calibration because of the consistency it gives with known population totals. As outlined in Chapter 5, the existing soft calibration methodology has its flaws and is likely to explain the lack of use in practice.

An interesting area for future work is to develop both the soft calibration problem and mean square error calibration simultaneously. Both are interesting areas of research in their own right, and shall be considered separately for the purpose of this thesis. However, there is certainly scope to bring these two approaches to calibration together. A brief explanation of how this can be done will be described in Section 6.4.

Recall that in the process of calibration, the weights $W$ have to stay as close as possible to the initial weights $D$. This is generally a practical requirement, since time is spent ensuring that the initial weights $D$ adjust for biases and non-response appropriately. To measure the closeness of $W$ and $D$, it is customary to use calibration functions of the form

$$\Phi(W) = \Phi(w_1, \ldots, w_n) = \sum_{i=1}^{n} q_i \phi(w_i), \qquad (30)$$

where $\phi(\cdot)$ is a univariate, strictly convex function with $\phi(d_i) = 0$ and $q_1, \ldots, q_n$ are given non-negative numbers; typically, $q_i = 1$ for all $i$. In this case, the function $\Phi$ is assessing the deviation between the calibrated weights $W$ and the initial weights

$D$. It is not uncommon to see these functions expressed as $\Phi(W, D)$ in existing literature. However, as the initial weights are considered fixed, the function $\Phi$ is simply a function of the calibrated weights $W$.

The function (30) plays the role of the objective function in the calibration optimization problem. Hard calibration can be written as the following optimization problem:

$$\Phi(W) \to \min_{W \in \mathbb{W}}, \text{ where } \Phi(\cdot) \text{ and } \mathbb{W} \text{ are defined in (30) and (28), respectively.} \tag{31}$$

Soft calibration can be written as the following optimization problem:

$$\Phi(W) \to \min_{W \in \mathbb{W}_1}, \text{ where } \Phi(\cdot) \text{ and } \mathbb{W}_1 \text{ are defined in (30) and (29), respectively.} \tag{32}$$

These optimization problems will be fully defined if we specify the function $\phi$ in (30). There are two natural conditions on the function $\phi$ in (30) (as given in [20]):

(a) $\phi(\cdot)$ is twice differentiable and strictly convex on its domain;

(b) $\phi(d_i) = 0$, $\phi'(d_i) = 0$, where the derivatives are taken with respect to the argument of the function $\phi(w)$.

The first of these conditions guarantees that the function is 'well-behaved' and has a minimum at the initial weights. The second condition requires that the function is 0 at the initial weights, since there is no deviation between the calibrated and initial weights in this case. Requiring the derivative to be zero at the initial weights also guarantees that there is a stationary point at these values, and due to the twice differentiability and strict convexity of the function, it is guaranteed to be a minimum.

The choices of the function $\phi$ have been discussed in detail in Chapter 4. However, in this chapter, only existing calibration functions shall be considered. This is to allow direct comparisons between the new approach and existing software packages, including the SAS Macro CALMAR [33] and the 'sampling' package in R [61].

The following three functions $\phi$ are implemented in many of the software packages and shall be considered throughout this chapter:

(i) Quadratic:

$$\phi^{(Q)}(w) = \frac{(w-d)^2}{2d};$$

(ii) Raking:

$$\phi^{(R)}(w) = w \ln\left(\frac{w}{d}\right) - w + d;$$

(iii) Logit:

$$\phi^{(L)}(w) = \frac{1}{C}\left[(w-ld)\ln\left(\frac{w-d}{d-ld}\right) + (ud-w)\ln\left(\frac{ud-w}{ud-d}\right)\right];$$

where $C = \frac{u-l}{(1-l)(u-1)}$.

In order to derive the new mean square error calibration methodology, the bias and variance of the calibration estimator is required. Before this can be done, let us revisit the notions of design-based and model-based sampling.

As described in Chapter 1, *model-based* sampling relies on a specific underlying probability model that describes the random process to generate the data. There are many possible choices for this model. Since we consider the model as a process for generating the data, it is possible to make conclusions that can be generalized to other data generated using the same process. However, a model can only ever approximate the true data. It is often difficult to truly know how deviations from the model will affect the analysis.

Analysis in survey sampling however is usually *design-based*. In this case, the population is pre-specified and data values for the population are considered to be fixed, rather than random. The observed sample is instead considered random, since the sample is generated by selecting individuals randomly from the fixed population. Since the random selection of individuals, referred to as the sample design, can be controlled, the probabilities of selecting individuals can often be known exactly. Design-based sampling uses the sample members to derive estimates of the fixed population. In the design-based framework, one cannot generalize the results of the inference to other populations.

Recall that sampling methods form the basis of design-based inference. Examples include simple random sampling, stratified sampling and cluster sampling. Any sampling method should satisfy the following conditions [35]:

- All individuals in the population have a non-zero probability of being selected in the sample. For individual $i$ we denote this probability by $\pi_i$.
- The probability $\pi_i$ must be known for every individual in the population, even those who do are not in the selected sample.
- Every pair of individuals must have a non-zero probability of both being in the sample. For individuals $i$ and $j$ we denote this probability as $\pi_{ij}$.
- The probability $\pi_{ij}$ must be known for every pair of individuals in the population, even those who do are not in the selected sample.

Suppose that we work in the design-based framework, but introduce a model that considers the relationship between the variables in the survey. In computing estimates and standard errors, we do not consider the goodness of fit of the model. However, the gain in precision from using the model is inevitably dependent upon the model's fit.

*Model-assisted inference* is the term used to describe estimation that is valid regardless of model fit, and efficient when the model fits well. The model is often referred to as a working model, which is a term also used in longitudinal data analysis (see, for example, [66]). The use of this term indicates that there is no assumption that the model is accurate, rather that the model is a practical tool that can be used to get more precise estimates.

To summarise, there are three approaches to sampling: design-based, model-based and model-assisted. An informal summary of each of these is given below.

**Design-based sampling:** the randomness is only attributed to the sampling variation. Observations are assumed to be fixed, and the only error is attributed to the sampling.

**Model-based sampling:** the variability in observations can be explained by a model, where the model variance can be split between observation errors and sampling errors.

**Model-assisted sampling:** one works in the design-based framework, however a model is introduced for purposes of estimation and computing standard errors that can be used to derive results regarding bias and variance. Estimators are valid regardless of model fit, and efficient when the model fits well.

In this chapter, a new approach to survey calibration is proposed that seeks to minimize the mean square error of the calibration estimator. In order to do this, the formulae for the variance and bias of the calibration estimator need to be derived. This enables us to formulate our approach in terms of both hard and soft calibration.

In Section 6.2, the variance and bias of the calibration estimator is derived. Mean square error calibration for hard constraints shall be predominantly described in this chapter, and outlined in Section 6.3. A brief overview of how this new method could be used for soft constraints is given in Section 6.4.

## 6.2 Bias and Variance of the Calibration Estimator

Working in the "model-assisted" framework, assume there is a model relating the variable of interest, $Y$, to the auxiliary variables $X$. This will allow the derivation of results regarding variance and bias. Remember that, in the model-assisted framework, the model does not have to be correct. The following model shall be assumed:

$$Y = X\theta + \varepsilon,$$

where $\mathbb{E}(\varepsilon) = \mathbf{0}_n$ and $\mathbb{D}(\varepsilon) = \sigma^2 V$, where $V$ is some (usually diagonal) matrix to be specified. For simplicity, a linear regression model has been assumed. There is scope to consider more complicated models, but that remains an area for further research.

Two possible cases for the matrix $V$ shall be considered:

- $V_d = \text{diag}(q_1 d_1, \ldots, q_n d_n)$, where $d_i$ denotes the $i$th initial weight,
- $V_w = \text{diag}(q_1 w_1, \ldots, q_n w_n)$, where $w_i$ denotes the $i$th calibrated weight,

and $q_i$, $i = 1, \ldots, n$, are arbitrary constants (usually set to 1). Both of these matrices have been suggested in existing literature (see for example [19] and [20]). The benefit of the first of these forms is that it only requires knowledge of the initial weights. The second matrix contains the calibrated weights, which are themselves derived as part of the process. This makes the calculations more challenging and complex.

Recall that $\pi_i$ denotes the inclusion probability of the $i$-th member of the sample, and $\pi_{ij}$ denotes the joint inclusion probability of the $i$-th and $j$-th sample members. The inclusion probability is defined to be the sum of probabilities for each sample that sample member $i$ will be selected for, whilst the joint inclusion probability is the sum of probabilities for the samples that members $i$ and $j$ will both be selected for. Let $E$ be an $n \times n$ matrix with entries $E_{ij} = \frac{\pi_{ij} - \pi_i \pi_j}{\pi_{ij}}$, $(i, j = 1, \ldots, n)$.

There is no known exact formula for the variance of the calibration estimator. This is due to the design-based nature of survey sampling. However, according to Deville et. al (1992), a model-assisted estimator of the variance of $Y'W$ is given by:

$$\text{Var}(Y'W) = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{(\pi_{ij} - \pi_i \pi_j)}{\pi_{ij}} (w_i e_i)(w_j e_j) = \tilde{W}' E \tilde{W}, \tag{33}$$

where $e_i = y_i - \mathbf{x}_i \hat{\theta}$, $\hat{\theta}$ satisfies the normal equations:

$$(X'VX)\hat{\theta} = X'VY,$$

and $\tilde{W}$ has elements $\tilde{w_i} = w_i e_i$ for $i = 1, \ldots, n$.

In the case $V = V_d$, the regression coefficients $\hat{\theta}$ do not depend on the calibrated weights $W$. However, in the case $V = V_w$, observe that $\hat{\theta}$, and therefore $e_i$, depends on the calibrated weights $W$. Let $\hat{\theta}_d$ denote the regression coefficients in the case $V = V_d$. In the case $V = V_w$, we shall write $\hat{\theta}_w$, to indicate the dependence of $\hat{\theta}$ on $W$.

Let $\mathbb{E}_M$ denote expectation with respect to the model, whilst $\mathbb{E}_D$ denotes expectation with respect to the sampling design. The total expectation, $\mathbb{E}$, is then defined as $\mathbb{E}_M\mathbb{E}_D = \mathbb{E}_D\mathbb{E}_M$. Note that we can always interchange the expectation when the model and design are independent of each other.

Let us now consider the bias of the estimator $Y'W$, assuming hard constraints of the form $X'W = T_X$:

$$\begin{aligned}\mathbb{E}(Y'W - T_Y) &= \mathbb{E}_D\mathbb{E}_M[Y'W - T_Y] \\ &= \mathbb{E}_D(W'X\theta) - T_Y \\ &= \mathbb{E}_D(W'X)\theta - T_Y \\ &= T_X'\theta - T_Y.\end{aligned}$$

For soft calibration, the constraints are of the form $X'W \approx T_X$. Therefore, the expression above gives the approximate bias in the case of soft calibration.

Having obtained expressions for the variance and the bias of the calibration estimator, we can now derive the mean square error. Recall that the mean square error is the sum of the variance and the square of the bias. In the following sections methods for minimizing the mean square error of the calibration estimators in the case of hard and soft constraints shall be derived.

## 6.3 Mean Square Error Calibration for Hard Constraints

In the previous section, it was shown that the variance of the calibration estimator is given by $\tilde{W}'E\tilde{W}$, where $\tilde{W}$ has elements $\tilde{w}_i = w_ie_i$ for $i = 1, \ldots, n$ and the $e_i$ are the errors derived from the assisting regression model. Recall that the matrix $E$ has entries $E_{ij} = \frac{\pi_{ij}-\pi_i\pi_j}{\pi_{ij}}$

This chapter makes use of the following result.

**Definition 6.1** (**Mean Square Error).** Let $\theta$ be an unknown parameter and suppose that $\hat{\theta}$ is an estimator of $\theta$. The mean square error, MSE, of the estimator $\hat{\theta}$ is given by

$$\mathrm{MSE}(\hat{\theta}) = \mathrm{Var}(\hat{\theta}) + (\mathrm{bias}(\hat{\theta}))^2.$$

Recall that there are two possibilities for the matrix $V$ where $\mathbb{D}(\varepsilon) = \sigma^2 V$. Either $V_d = \text{diag}(q_1 d_1, \ldots, q_n d_n)$, where $d_i$ denotes the $i$th initial weight, or $V_w = \text{diag}(q_1 w_1, \ldots, q_n w_n)$, where $w_i$ denotes the $i$th calibrated weight. Mean square error calibration for hard constraints shall be considered in both of these cases.

**Case 1:** If $V = V_d$, then the estimate of $\theta$ is $\hat{\theta}_d$ and the resulting estimate of the bias is:

$$\text{bias}(Y'W) = T'_X \hat{\theta}_d - T_Y.$$

Note that this does not depend on the calibrated weights $W$. Therefore, the weights that minimize the variance will be equivalent to those that minimize the mean squared error. So in this case, the bias does not need to be considered as part of the mean square error calibration.

Recall that the feasibility domain for the hard calibration problem is given by $\mathbb{W} = \{W = (w_1, \ldots, w_n)' : \ L \circ D \leq W \leq U \circ D \text{ and } X'W = T_X\}$. Using this, we can state the calibration problem as follows:

$$W'EW \to \min_{W \in \mathbb{W}}. \tag{34}$$

**Case 2:** If $V = V_w$, then the estimate of $\theta$ is $\hat{\theta}_w$ and in this case the estimate of the bias is given by:

$$\text{bias}(Y'W) = T'_X \hat{\theta}_w - T_Y.$$

Note that this does depend on the calibrated weights $W$. Therefore, it needs to be considered as part of the calibration problem. Using (28), the calibration problem can be stated as follows:

$$W'EW + (T'_X \hat{\theta}_w - T_Y)^2 \to \min_{W \in \mathbb{W}}. \tag{35}$$

Several examples shall now be considered to explore the behaviour of the calibration problems described above. Case 2 is computationally challenging to implement and still require further investigation. Therefore, unless otherwise stated, only case 1 shall be considered in the examples that follow.

### 6.3.1 Simulation Example

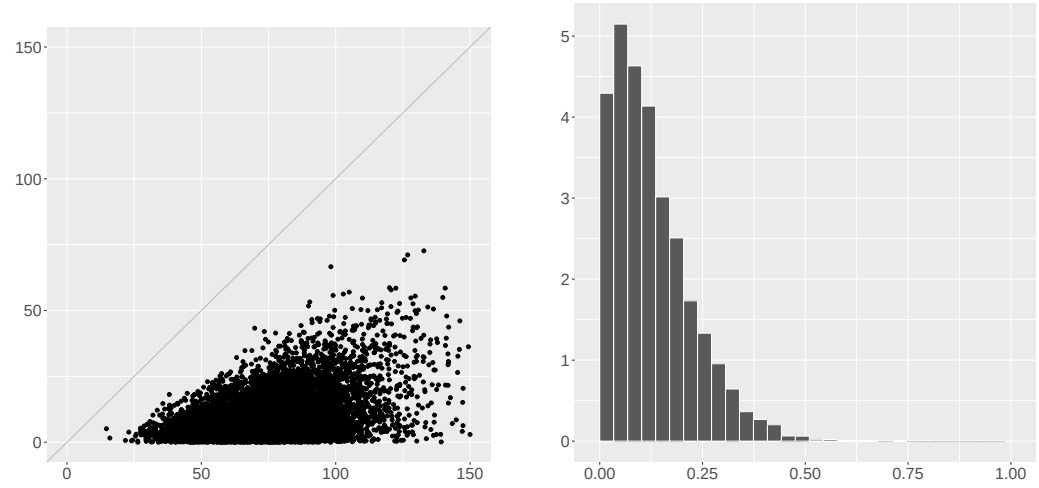
In this example, the population has size $N = 100$, and 10,000 simple random samples of size $n = 20$ are taken. Random vectors $X$ and $Y$ are generated, both from a normal distribution, such that the correlation between $X$ and $Y$ is 0.9.

The non-negativity constraint $w_i \geq 0$ is imposed throughout. Results are compared from classical calibration using the quadratic function $\phi^{(Q)}$ (classical method 1, denoted CM1), with the calibrated weights using (34) (alternative method 1, denoted AM1) and (35) (alternative method 2, denoted AM2). The MSE and variance of the estimator $Y'W$ are compared in both cases.

In Figures 31, the variance of the estimator $Y'W$ for AM1 and the variance of the estimator using CM1 are compared. A scatter plot of the variance of $Y'W$ using AM1 against the variance of $Y'W$ using CM1 is given in Figure 31(a). The ratio of the variance of $Y'W$ using AM1 to the variance of $Y'W$ using CM1 is given in Figure 31(b). Similarly, Figure 32 compares the MSE of the estimator $Y'W$ using methods CM1 and AM2. Figure 32(a) shows a scatter plot of the MSE of the estimator $Y'W$ using weights from AM2 against the MSE of the estimator using weights from CM1. Figure 32(b) shows a histogram of the ratio of the MSE of $Y'W$ using AM2 to the MSE of $Y'W$ using CM1.

Observe in both scatter plots that all the points lie under the main diagonal, and the ratio of the variances/MSE in the histograms is between 0 and 1. Hence, the variance is always smaller using the AM1 than using CM1, and the MSE is always smaller using AM2 than using CM1. These graphs confirm that the methods have worked and have found a calibration estimator with smaller variance/mean square error. This is of course to be expected, since the weights derived using AM1 were obtained using the mean square error as the optimization criteria. Further investigation is needed to compare these methods according to other suitable measures. Examples could include the reliability of estimates and the distribution of the derived calibrated weights. This remains an area for further investigation.

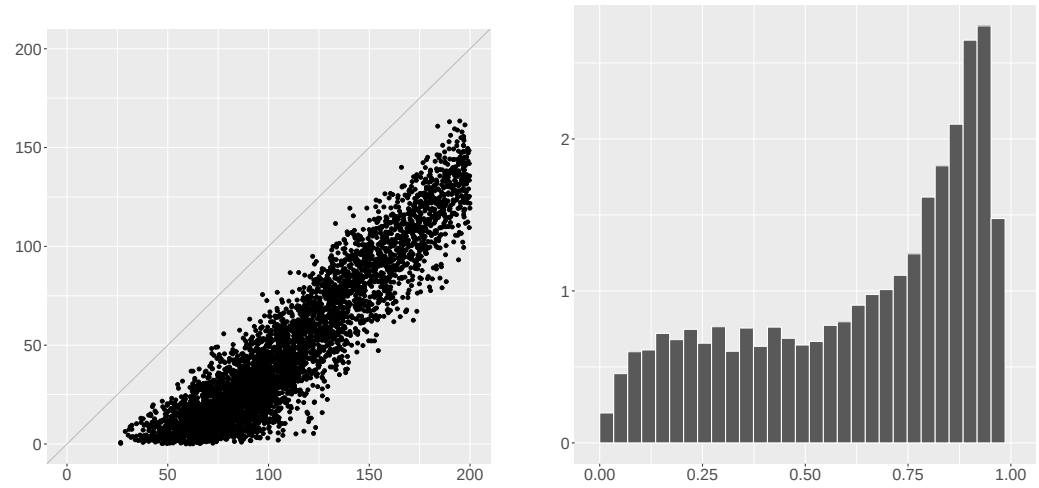
For this example, similar results were obtained when comparisons were made with other calibration functions. Therefore, additional scatter plots and histograms are




(a) Scatter plot of variance using AM1 against variance using CM1

(b) Histogram of ratio of variance using AM1 to variance using CM1

Figure 31: Comparison of variance of the estimator $Y'W$ when using AM1 and CM1




(a) Scatter plot of MSE using AM2 against MSE using CM1

(b) Histogram of ratio of MSE using AM2 to MSE using CM1

Figure 32: Comparison of MSE of the estimator $Y'W$ when using AM2 and CM1

not included here. This example has confirmed that the methodology correctly finds calibration estimators with smaller variance/MSE. In the next example, the behaviour of alternative method 1 (AM1) is compared with classical calibration approaches for various sampling methods. The alternative method will be shown to always give estimators that have smaller variance/mean squared error.

### 6.3.2 California Academic Performance Index (API) Example

In this example, the Academic Performance Index (API) datasets included as part of the 'survey' package in R (see [36] for more details) shall be considered. The data sets include information about the academic performance index for 6194 schools in California in 1999 and 2000. The academic performance index is calculated from standardized tests that are taken by all students in elementary, middle and high schools in California.

The first data set, 'apipop', contains all schools in California with at least 100 students. The second dataset, 'apisrs', contains a simple random sample of 200 of the 6194 schools from the 'apipop' dataset. The third dataset, 'apistrat', contains a stratified sample of 200 schools stratified by school type (elementary, middle and high).

For the fourth dataset, 'apiclus1', the 757 school districts within California are treated as clusters. The apiclus1 dataset contains the 183 schools that are in 15 randomly selected school districts (clusters). Finally, the 'apiclus2' dataset contains 126 schools that were obtained through two-stage cluster sampling. For the two-stage cluster sample, 40 school districts (clusters) were selected at random, with random samples being taken within each cluster.

The purpose of the calibration is to estimate the total number of students that were tested in the 1999-2000 academic year. Within each of the datasets, the variable api.stu gives the number of students that were tested at each school. The auxiliary variables in this example will be school type. Therefore the columns of $X$ are vectors of 0s and 1s, where $x_{ij} = 1$ if school $i$ is type $j$ ($j = 1, 2, 3$), and $x_{ij} = 0$ otherwise.

For these datasets, the performance of the mean square error calibration shall be investigated for various sampling schemes, namely simple random sampling (SM1), stratified sampling (SM2), cluster sampling (SM3) and two-stage cluster sampling (SM4).

For each of these sampling methods, the variance of estimates obtained using mean square error calibration shall be compared with weights derived using four classical calibration methods:

- Calibration Method 1 (CM1): Quadratic, no weight bounds,
- Calibration Method 2 (CM2): Raking, non-negativity bounds,
- Calibration Method 3 (CM3): Quadratic, $l_i = 0.25$, $u_i = 4$ for $i = 1, \ldots, n$,
- Calibration Method 4 (CM4): Logit, $l_i = 0.25$, $u_i = 4$ for $i = 1, \ldots, n$,

The table below gives the ratio of the variance of estimates using mean square error calibration with the variance of estimates using classical calibration methods.

| Methods | CM1 | CM2 | CM3 | CM4 |
|---|---|---|---|---|
| SM1 | 0.843 | 0.812 | 0.838 | 0.838 |
| SM2 | 0.639 | 0.565 | 0.606 | 0.606 |
| SM3 | 0.715 | 0.679 | 0.695 | 0.695 |
| SM4 | 0.682 | 0.623 | 0.645 | 0.645 |

Table 13: Ratio of variance of the calibration estimator using classical calibration methods to the variance of the calibration estimator using the new method for various sampling methods (SM) and calibration methods (CM).

Observe that all the ratios in Table 1 are less than 1. Therefore, for every sampling method and classical calibration method, mean square error calibration has resulted in estimates with smaller variance. This again indicates the success of the methodology in finding calibration estimators with smallest mean square error. This example has simply demonstrated that mean square error calibration works. Comparing these methods using other criteria, such as the distribution of the calibrated weights, should also be conducted and remains an area for further research.

The final example in this section shall explore the impact of adding additional calibration variables to the model. The examples considered so far have only had one auxiliary variable. Additional auxiliary variables shall be added to the model and the mean square error of the resulting estimates considered.

### 6.3.3 Belgian Municipalities Example

Again, consider the Belgian municipalities dataset included in the 'sampling' package in R, as used for the example in Section 6.3.1. Recall that the data provides information about the Belgian population at July 1st 2004 compared with July 1st 2003 and includes some financial information about the municipality incomes at the end of 2001. Data is available for the 589 municipalities in Belgium. There are 17 variables in the dataset including the municipality name and province number. However, the 4 variables of interest in this example are the number of men on July 1st 2003, the number of women on July 1st 2003, total taxable income in Euros in 2001, and total taxation in Euros in 2001.

The purpose of this example is to investigate the impact of adding additional calibration variables to the model. In the simple example of Section 6.3.1, only one auxiliary variable was considered. This section begins by considering two variables, namely the number of males in 2003 and the number of females in 2003. For the population data, these two variables proved significant in a multiple linear regression model. The variables for total taxable income and total taxation shall then be added. These variables were not significant in the multiple linear regression model.

Taking 1,000 simple random samples of size 50 and assign initial weights as $d_i{=}N/n$ where $N$ is the size of the population and $n$ is the sample size (in this example $N = 589$ and $n = 50$). These would be the weights used in the Horvitz-Thompson estimator [28]. The values of the variables of interest for each of the 50 sample members are used to form the $50 \times m$ matrix $X$, where $m$ denotes the number of variables included in the calibration model. Here, the cases $m = 2$ and $m = 4$ are considered.

Each sample shall be calibrated using the following classical calibration approaches:

- Classical Method 1 (CM1): Quadratic function $\phi^{(Q)}$, no weight bounds.
- Classical Method 2 (CM2): Raking function $\phi^{(R)}$, non-negativity bounds.

- Classical Method 3 (CM3): Quadratic function $\phi^{(Q)}$, $l_i = 0.25$, $u_i = 4$ for $i = 1, \ldots, n$.
- Classical Method 4 (CM4): Logit function $\phi^{(L)}$, $l_i = 0.25$, $u_i = 4$ for $i = 1, \ldots, n$.

In this section, the following methods are also considered:

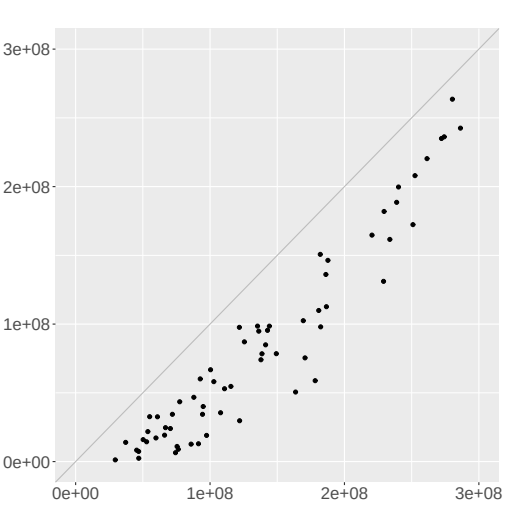
- Alternative Method 1 (AM1): Solving (34) with no weight bounds.
- Alternative Method 2 (AM2): Solving (34) with non-negativity bounds.
- Alternative Method 3 (AM3): Solving (34) with $l_i = 0.25$, $u_i = 4$ for $i = 1, \ldots, n$.

Firstly consider $m = 2$. Therefore, there are two auxiliary variables, namely the number of males in 2003 and the number of females in 2003. In Figure 33, the MSE of the estimator $Y'W$ using weights from the AM1 against the MSE using CM1 is plotted. A histogram of the ratio of the MSE for the estimator using AM1 to the MSE using CM1 is also given. Similarly, Figure 34 plots the MSE of the estimator $Y'W$ using weights from AM2 against the MSE using weights from CM2. A histogram of the ratio of the MSE of the estimates using AM2 to the MSE when using CM2 is also provided.

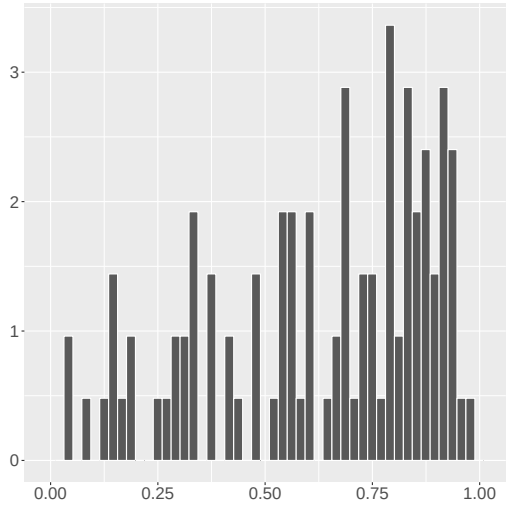
For $m = 2$, similar pictures for comparisons of AM1, AM2 and AM3 against the classical methods with corresponding weight bounds can be derived. In all cases, they show that mean square error calibration gives estimates with smaller variance/mean square error.

Now consider $m = 4$, meaning there are four auxiliary variables. These are: the number of males in 2003, the number of females in 2003, total taxable income in 2001 and total taxation in 2001. Recall that two of these variables, namely total taxable income and total taxation, were not significant when a multiple linear regression was run.

In Figure 35, the variance of the estimator $Y'W$ using weights from AM1 is compared with the MSE using weights from CM1. Scatter plots of the variances, and a histogram of the ratio of the variances are given. Again, comparisons

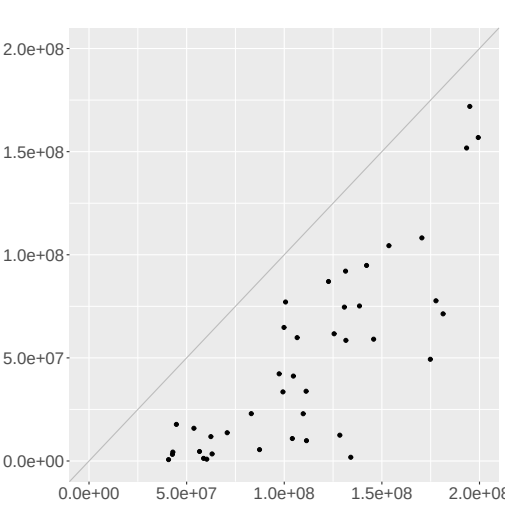



(a) Scatter plot of MSE using AM1 against MSE using CM1

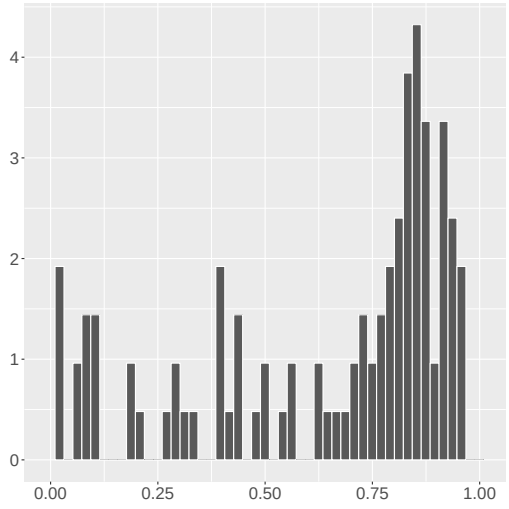



(b) Histogram of ratio of MSE using AM1 to MSE using CM1

Figure 33: Comparison of MSE of $Y'W$ when using AM1 and CM1 ($m = 2$)



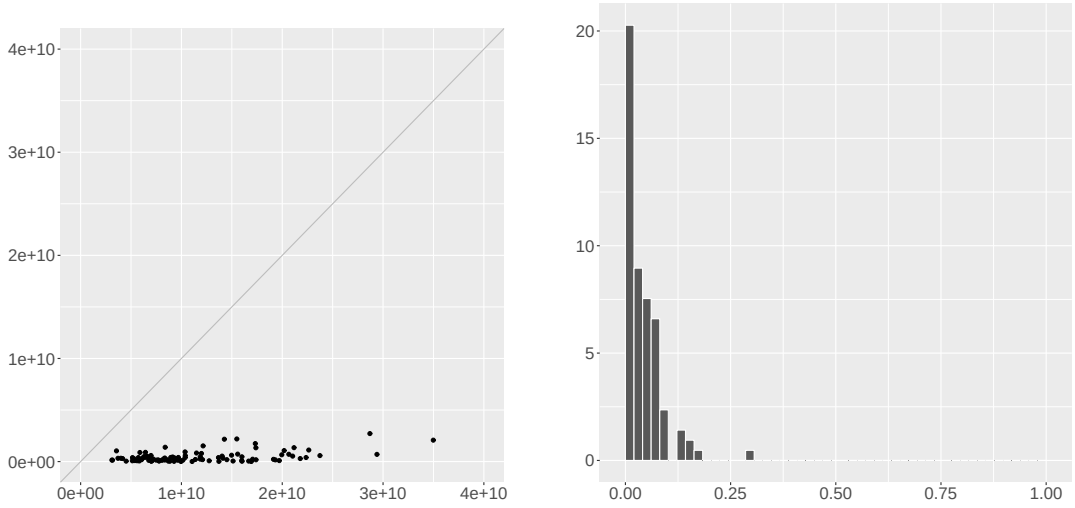

(a) Scatter plot of MSE using AM2 against MSE using CM2




(b) Histogram of ratio of MSE using AM2 to MSE using CM2

Figure 34: Comparison of MSE of the estimator $Y'W$ when using AM2 and CM2 ($m = 2$)

of AM1, AM2 and AM3 against the classical methods with corresponding weight bounds gave similar scatter plots and histograms. Therefore, they are not included here.




(a) Scatter plot of MSE using AM1 against MSE when using CM1

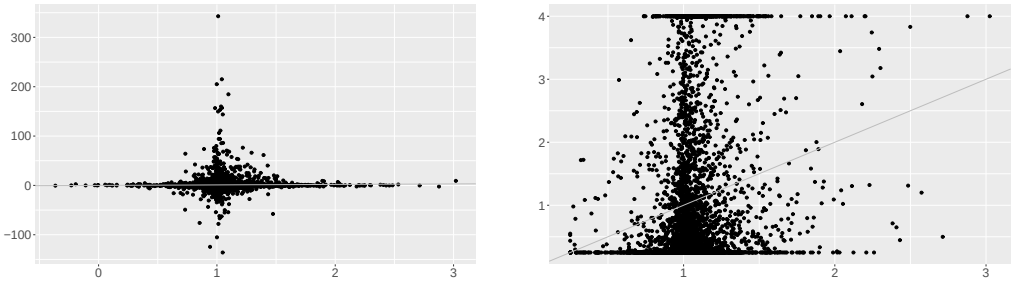
(b) Histogram of ratio of MSE using AM1 to MSE using CM1

Figure 35: Comparison of MSE of the estimator $Y'W$ when using AM1 and CM1 ($m = 4$)

So far, the weights from mean square error calibration have not been considered. These are now compared with the weights from classical calibration. In Figure 36(a), the weights from AM1 are plotted against the weights from CM1. The scatter plot shows that the weights from AM1 are far more variable than the weights from classical calibration.

In Figure 36(b), the weights from AM3 are compared with the weights from CM3. More of the weights approach the boundary values of 0.25 and 4 in the case of AM3, compared to the weights from CM3 that are more clustered around 1.

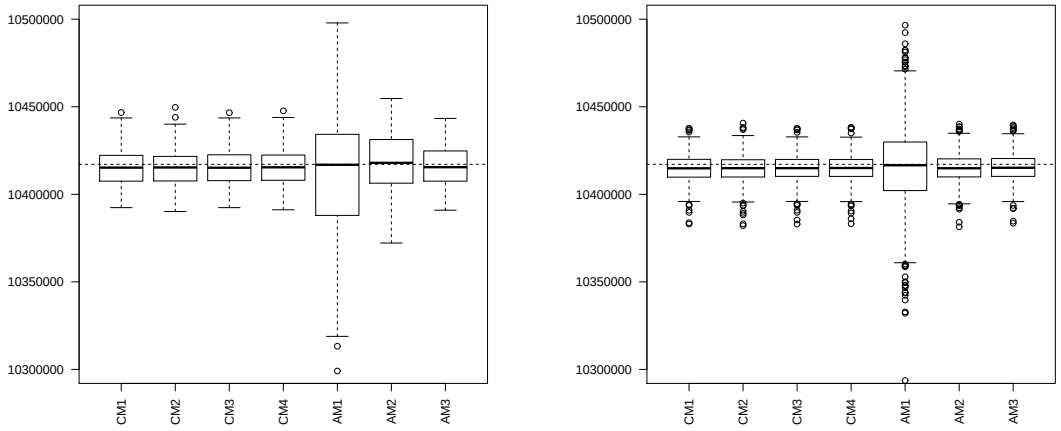
In Figure 37, the distribution of the estimates $Y'W$ is given for each of the four classical calibration methods, and the three alternative methods. The estimates for $m = 2$ are given in Figure 37(a) and the estimates for $m = 4$ are shown in Figure 37(b). In both figures, we see that the estimates for AM1 and AM2 are far more variable than the estimates using CM1 and CM2, respectively. This is counter-intuitive, since our objective with this method is to minimize the mean squared error of the estimates. Similarly, there is very little difference in the variability of the estimates from AM3 compared to the estimates using CM3 and CM4.




(a) No weight constraints (b) Bounded weight constraints

Figure 36: Scatter plot of calibrated weights using the alternative approach against calibrated weights using classical methods in various weight constraint cases

Further study is needed to investigate the causes of this. There is a contradiction here, since the variance and mean square error are smaller according to the formulae given in 6.3. However, as we have seen in the histograms in Fig. 37, there is a much greater variability in the estimates from this method, compared to the estimates from classical calibration.




(a) Histogram of $Y'W$ in the case $m = 2$ (b) Histogram of $Y'W$ in the case $m = 4$

Figure 37: Distribution of $Y'W$ for the case $m = 2$ and $m = 4$ for various calibration methods

Mean square error calibration is still a relatively new methodology. It has been shown in these examples to significantly reduce the mean square error of the

estimates, however there is still much scope for further comparisons with existing methodologies to highlight the key benefits of this method.

In the next section, a brief overview of how mean square error calibration can be conducted in the case of soft constraints is given.

## 6.4 Mean Square Error Calibration for Soft Constraints

By relaxing the constraint $X'W = T$, we can define the soft feasibility domain $\mathbb{W}_1 = \{W = (w_1, \ldots, w_n)' : \ L \circ D \leq W \leq U \circ D \text{ and } X'W \simeq T_X$. Again, two cases are considered depending on the form of the matrix $V$.

**Case 1:** If $V = V_d$, the bias is constant with respect to $W$. Therefore, it is not included in the calibration problem, which can be stated as follows:

$$W'EW + \beta^{-1}(X'W - T)'C(X'W - T) \to \min_{W \in \mathbb{W}_1}, \tag{36}$$

where $C$ is a diagonal matrix (often taken to be the identity matrix), and $\beta$ is some chosen constant.

**Case 2:** If $V = V_w$, the bias does depends on the calibrated weights $W$. Therefore, in this case, the calibration problem can be stated as follows:

$$W'EW + (T_X'\hat{\theta}_w - T_Y)^2 + \beta^{-1}(X'W - T)'C(X'W - T) \to \min_{W \in \mathbb{W}_1}, \tag{37}$$

where $C$ is a diagonal matrix (often taken to be the identity matrix), and $\beta$ is some chosen constant.

More investigation is needed for this approach, and the suitability of using the approximate bias requires further study. However, it remains an interesting area of future investigation to combine mean square error calibration with soft calibration.

## 6.5 Summary

In this chapter, a new approach to the calibration problem has been presented. This aims to minimize the mean square error of the calibration estimator directly, whist satisfying the calibration constraints either exactly or approximately.

This is still a relatively new area of research, and there is scope for further development and improvement of the methodology. Further comparisons with existing methods is also needed to truly highlight benefit of this new approach.

In the next chapter, the findings from this thesis are summarised and areas for future research considered.

# 7 Conclusion and Further Work

This research has investigated the calibration problem and developed several methods for solving this key official statistics problem. As well as building on existing methodologies, it has also introduced a new approach to calibration based on the practical requirements of the calibration estimator. This chapter will present a summary of the key findings and conclusions that can be drawn from the research. It also outlines the contributions made to the field and identifies areas for future research.

This chapter is structured as follows. Section 7.1 concludes the research presented in this thesis and provides a summary of each of the chapters. Section 7.2 outlines areas for further investigation and future research questions based on this research. Section 7.3 provides some closing remarks to the thesis.

## 7.1 Conclusion

This research has provided a unified theory for describing the calibration problem through use of optimization. Several new calibration functions have been presented, with their benefits described. We have also explored the use of soft calibration, presenting the drawback with existing approaches and describing soft calibration's potential as a constraint diagnostic tool. A new method for calibration has also been proposed that involves direct minimization of the mean squared error of the calibration estimator.

An overview of each chapter is given, with the main conclusions and contributions that can be drawn from each chapter.

**Chapter 1** described the benefits of calibration problem and highlighted several practical considerations when using calibration. This provided the motivation for the research presented in this thesis. The two main approaches to calibration, namely hard calibration and soft calibration, were also presented.

**Chapter 2** outlined a new framework for calibration, namely calibration as an optimization problem. Whilst many authors have described the calibration problem, they have not done so via optimization.

**Chapter 3** explored several algorithms and software packages currently used to perform calibration. This research described these algorithms mathematically, and highlighted some of the flaws in existing calibration software.

**Chapter 4** provided a critical analysis of existing calibration functions and introduced two new calibration functions that improve upon those that are currently implemented.

**Chapter 5** described soft calibration, firstly via optimization as a method for solving the calibration problem. Whilst appealing since it guarantees a solution to the calibration problem, it is unlikely to be adopted in practice due to the relaxing of the calibration constraints (albeit slight in most cases). However, a clear practical use for soft calibration is as a diagnostic tool for identifying problematic calibration constraints.

**Chapter 6** presented a new approach to calibration that directly minimizes the mean square error of the calibration estimator. This has practical appeal, since the variance of the calibration estimator has a relative importance to practitioners.

In the next section, we explore ways in which the research in this thesis can be extended. We consider both theoretical extensions of this research, as well as practical considerations for implementation of the findings in this thesis.

## 7.2 Further Work

Inevitably, there is scope for further work and extensions to the research presented in this thesis. Opportunities for future research associated with this thesis are outlined in this section.

In this thesis, we focused on the classical calibration problem and its formulation in terms of optimization. However, there is a vast literature on calibration with many

methods not considered in this thesis. An interesting area for future investigation is the use of the optimization framework to describe these methods. Optimization is likely to provide a standardized approach through which many other calibration methods can be described. This would bring together many approaches under one standard theory.

Several new calibration functions have been presented in Chapter 4. These were motivated primarily from the practical use of reducing the number of calibration weights that cluster at the bounds. There is scope to further explore the theoretical properties of these functions, as well as using them as part of soft calibration as described in Chapter 5.

The work in Chapter 3 mainly provided a critical analysis of the existing algorithms and software. An interesting area for further research is extending these algorithms to include the new calibration functions presented in Chapter 4. Furthermore, as calibration can be considered as an optimization problem, there is scope to experiment with various alternative optimization algorithms.

Soft calibration has received far less attention in calibration literature, and national statistical offices are reluctant to use this approach as a calibration method. However, it guarantees a solution to the problem, and leads to virtually the same solution as hard calibration in the majority of cases. Through further research, the optimization approach to soft calibration proposed in this thesis can be extended and its practical use further explored.

Whilst this thesis focused on quadratic functions for soft calibration, the functions presented in Chapter 4 could also be incorporated as part of the problem. Experimenting with various choices of the two soft calibration functions remains an area for further investigation.

An alternative practical use of soft calibration is as a diagnostic tool. This allows those performing calibration to identify the 'challenging' constraints. There has been interest from the Office for National Statistics to incorporate this method as part of their 'library of methods' for analysing survey data. Development of this methodology with the ONS is an interesting area for future collaboration.

The new approach of mean square error calibration is still in its early stages of development. Whilst practically appealing for leading to reduced mean square error of the calibration estimator, there is scope for further investigation of the estimates obtained using this approach. The mean square error calibration presented in this thesis only considered 'hard calibration' constraints. There is arguably still much work needed to further develop and extend the theoretical ideas presented in this thesis. A natural extension of this area of research is the combination of mean square error calibration with 'soft calibration' constraints.

## 7.3 Final Remarks

The research in this thesis has identified the importance of the calibration problem in the analysis of sample surveys. It is a vital tool in the analysis of offical statistics. Calibration is a method of providing consistency between surveys, reducing the variance of estimates and accounting for non-response or coverage bias. This thesis has focused on the first two of these motives for calibration.

In this chapter, we have outlined the significant findings from this research, which has included several alternative approaches to calibration in survey sampling. Areas for further research and investigation have been identified. There is scope for these methods to be adopted by national statistical offices, and the Office for National Statistics has played an important role in contributing to the practical viewpoint of this research. There is interest to adopt the methodologies presented in this research at the Office for National Statistics.

One of the key contributions of this thesis has been to present a unified framework for both the hard and soft calibration problems. Also, new calibration functions have been proposed, and a the methodology for soft calibration developed. Furthermore, a new calibration methodology has been introduced that minimizes the mean square error of the calibration estimator. Further research into both soft calibration and mean square error calibration presents an interesting scope for further research.

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