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Abstract: If part of a population is hidden but two or more sources are available that each cover parts of this population, dual- or multiple-system(s) estimation can be applied to estimate this population. For this it is common to use the log-linear model, estimated with maximum likelihood. These maximum likelihood estimates are based on a non-linear model and therefore suffer from finite-sample bias, which can be substantial in case of small samples or a small population size. This problem was recognised by Chapman, who derived an estimator with good small sample properties in case of two available sources. However, he did not derive an estimator for more than two sources. We propose an estimator that is an extension of Chapman's estimator to three or more sources and compare this estimator with other bias-reduced estimators in a simulation study. The proposed estimator performs well, and much better than the other estimators. A real data example on homelessness in the Netherlands shows that our proposed model can make a substantial difference.

Keywords: Finite sample bias, Log-linear model, Multiple-systems estimation, Chapman estimator

1 Introduction

A well-known statistical problem concerns the estimation of the size of a population that is only partly observed by different sources. By linking the records in the sources the number of units observed by at least one source is found, but the number of units that are missed by all sources is unknown. The standard method to estimate this hidden number is known as dual-system estimation (DSE) for two lists and multiple-systems estimation (MSE) for more than two lists. Other names found in the literature are *capturerecapture, mark-recapture, multiple-recapture* and *multiple-record systems* estimation. A literature overview is provided by Chao (2001), who discusses these models in the context of human populations.

DSE leans on a set of assumptions extensively described by, for example, Wolter (1986) and Zhang (2019). The International Working Group for Disease Monitoring and Forecasting (1995) summarize them as:

- 1. There is no change in the population during the investigation (the population is closed).
- 2. There is no loss of tags (individuals can be linked from capture to recapture).
- 3. For each sample, each individual has the same chance of being included in the sample.

4. The two samples are independent.

Earlier Seber (1982) and later Chao et al. (2001) and van der Heijden et al. (2012) showed that assumption 3 can be further relaxed, i.e., it is sufficient that each individual has the same chance of being included in only one of the samples, instead of both samples. In MSE, samples are allowed to be dependent, and in practical situations this makes MSE much more realistic than DSE.

Under the appropriate assumptions and conditions, a maximum likelihood (ML) estimator can be derived for the hidden and total population size. However, in finite samples these ML-estimators are mean-biased (see e.g. Bailey, 1951; Chapman, 1951; Rivest & Lévesque, 2001). This mean-bias can be shown for the ML-estimators directly, but also follows more generally from the fact that these estimators make use of a hierarchical loglinear model (Fienberg, 1972), which provides median-unbiased, but not mean-unbiased estimates (see e.g. Hald, 1952, chap. 7, or Miller, 1984). This finite-sample mean-bias (from now on referred to as finite-sample bias or simply bias) can be substantial in case of small samples (Long, 1997, p. 53-54; Rainey & McCaskey, 2021).

The role of finite-sample bias in the discussion on the robustness and accuracy of MSE estimators is generally small. The focus is usually on other issues that lead to inaccurate estimates, such as failing model assumptions (see e.g. Gerritse, van der Heijden, & Bakker, 1993; Zult, De Wolf, Bakker, & Van der Heijden, 2021) or model selection uncertainty (see e.g. Binette & Steorts, 2022; Silverman, 2020). While it is true that these issues can potentially lead to large estimation bias, it is not clear how these issues are affected by finite-sample bias, simply because it is usually ignored. This is unfortunate, because correcting for finite-sample bias comes at almost no costs to researchers (Rainey & McCaskey, 2021), while, as we will see, its impact can be substantial and therefore may affect conclusions.

The first to address the problem of finite-sample bias in DSE were Chapman (1951) and Bailey (1951). To reduce bias, they both proposed their own bias-reduced DSE estimator. Chapman showed that his estimator is essentially unbiased (Chapman, 1951, p. 145) and it became the most well-known of the two. Neither the Chapman nor Bailey estimator was extended towards MSE. The main contribution of this paper is the proposal of a Chapman MSE-estimator.

Our proposed Chapman MSE-estimator is not the first estimator that aims to reduce bias in the ML-estimator. Evans and Bonett (1994) and Rivest and Lévesque (2001) proposed population size estimators with the same goal. Others, such as Cordeiro and Mc-Cullagh (1991), Firth (1993) and Kosmidis and Firth (2021); Kosmidis, Kenne Pagui, and Sartori (2020), proposed bias-reduction methods for ML-estimators in log-linear models in general, which can be used in the context of MSE. In this paper we will compare the performance of these bias-reduced MSE estimators with our Chapman MSE-estimator in simulation studies.

The paper is structured as follows. Section 2 discusses DSE and bias in DSE estimators. Section 3 discusses MSE and a derivation of the new Chapman MSE-estimator for *saturated* log-linear models, i.e., log-linear models where the number of independent parameters equals the number of counts. In Section 3.3 this new estimator is generalised towards a Chapman MSE-estimator that is also valid for *restricted* log-linear models. In Section 4 the new Chapman MSE-estimator is used to estimate the number of homeless people in The Netherlands. Section 5 discusses and concludes.

2 Dual-system estimation

This section discusses DSE. We first introduce notation, then Section 2.1 proceeds with the Lincoln-Peterson estimator and the log-linear model. Section 2.2 discusses the different distributional assumptions that underlie DSE and some of their implications. Section 2.3 introduces the problem of mean-bias and gives the bias-reduced DSE estimators proposed by Chapman (1951) and Bailey (1951). This section also presents an alternative interpretation of the derivation of the Chapman-estimator that has the advantage that it allows the Chapman-estimator to be easily extended towards a similar estimator for multiple sources (which we will do in Section 3). Finally, in Section 2.4, bias-reduced DSE estimators are compared in a simple simulation study.

A description of the DSE problem starts from a population that consists of N unique units that are partly observed by two sources A and B, where the units are matched between sources. Each source is a random sample from the population, so in general not all N units are observed. Each unit has an inclusion pattern that tells us in which source(s) a unit was observed. This inclusion pattern is denoted as ab with a, b = 1, 0, where a = 1 stands for 'in the first source' and a = 0 for 'not in the first source', and the same with b for the second source. This implies that the inclusion pattern 00 belongs to the unobserved units.

DSE uses the frequencies of occurrence of each inclusion pattern, which are simply the counts of the units with identical inclusion patterns. These counts are denoted as n_{ab} . A vector of the observed counts is denoted as \mathbf{n} , excluding the unobserved count n_{00} that is unknown and to be estimated. When we sum over a or b, we replace that subscript by '+'. Thus $n_{10} + n_{11} = n_{1+}$ is equal to the size of the first source, and n_{+1} to the size of the second source. The total number of observed units is denoted as n, which allows us to write $N = n + n_{00}$. n_{ab} is considered a random variable with expectation m_{ab} . Estimates for N, m_{ab} and m_{00} are denoted by \hat{N}^{est} , $\hat{m}^{\text{est}}_{ab}$ and $\hat{m}^{\text{est}}_{00}$, where the superscript 'est' indicates the estimator that was used. These bias-reduced estimators can be obtained by using adjusted counts, that we denote as n^{est}_{ab} or \mathbf{n}^{est} .

2.1 The Lincoln-Petersen estimator and the log-linear model

The first DSE model for population size estimation was proposed by Petersen (1896), and later Lincoln (1930). It is often referred to as the Lincoln-Petersen (LP) estimator. The LP-estimator can be derived from the assumption of independence between source *A* and *B*,

which implies that the odds-ratio between source A and B, denoted by θ^{AB} , is

$$\theta^{AB} = \frac{m_{11}/m_{10}}{m_{01}/m_{00}} = 1,\tag{1}$$

which leads to

$$m_{00} = \frac{m_{10}m_{01}}{m_{11}}.$$
(2)

By plugging in ML estimates for m_{ab} , which are simply the observed values $n_{ab}^{\text{LP}} = n_{ab}$ (see e.g., Bishop, Fienberg, & Holland, 1975), the LP-estimator for the missing cell is

$$\hat{m}_{00}^{\text{LP}} = \frac{n_{10}^{\text{LP}} n_{01}^{\text{LP}}}{n_{11}^{\text{LP}}} = \frac{n_{10} n_{01}}{n_{11}},\tag{3}$$

and the population size estimate

$$\hat{N}^{\rm LP} = n + \hat{m}_{00}^{\rm LP} = \frac{n_{1+}n_{+1}}{n_{11}}.$$
(4)

The LP-estimator for the missing cell and for the population size are ML estimators.

Fienberg (1972) shows that the LP-estimator can also be obtained from log-linear parameter estimates of the log-linear model

$$\log \mathbb{E}\left[\mathbf{n}|\mathbf{X}\right] = \mathbf{X}\boldsymbol{\lambda},\tag{5}$$

with, for two sources,
$$\mathbf{n} = \mathbf{n}^{\text{LP}} = (n_{11}, n_{01}, n_{01})^{\top}$$
, $\mathbf{X} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$ and $\boldsymbol{\lambda} = (\lambda, \lambda_a^A, \lambda_b^B)^{\top}$.

 λ is the intercept term, and λ_a^A and λ_b^B are the respective inclusion parameters for source A and B that are identified by setting $\lambda_0^A = \lambda_0^B = 0$. It is further assumed that Eq. (5) also holds for m_{00} . The parameters of a log-linear model are usually estimated with ML, which for Eq. (5) gives the ML estimates $\hat{\lambda}^{ML}$, $\hat{\lambda}_a^{A,ML}$ and $\hat{\lambda}_b^{B,ML}$, which can be used to estimate m_{00} , i.e.:

$$\hat{m}_{00}^{\rm ML} = \exp{\hat{\lambda}^{\rm ML}},\tag{6}$$

where \hat{m}_{00}^{ML} is equal to \hat{m}_{00}^{LP} . It is well known that ML-estimators for log-linear models are biased (see e.g. Hald, 1952, chap. 7, or Miller, 1984), so this also holds for \hat{m}_{00}^{LP} .

2.2 Distributional assumptions

Chapman (1951) and Bailey (1951) showed that the LP-estimator can be derived as an MLestimator, assuming that n_{11} and n_{01} conditional on n_{1+} and N, follow a hypergeometric (Chapman) or binomial (Bailey) distribution. In the context of population size estimation, a hypergeometric distribution seems more fitting, because it assumes *sampling without replacement*, which matches the 'no duplicates' assumption (i) of Zhang (2019). Bailey(1951, p. 294) was aware of this issue when he wrote 'We shall assume that n_{+1} is sufficiently small compared with N for us to be able to ignore the complications of sampling without replacement'. However, later Darroch (1958) argued that this choice is less obvious. He first showed that the LP-estimator can also be derived by assuming either

$$(n_{11}, n_{10}, n_{01}, n_{00}) \sim Multinomial (N, p_{11}, p_{10}, p_{01})$$

or

$$(n_{11}, n_{10}, n_{01}, n_{00}) \sim$$
Hypergeometric $(N, p_{11}, p_{10}, p_{01})$

with $p_{ab} = m_{ab}/N$. Darroch (1958) discusses which of both distributions to any given experiment is the appropriate choice. He concludes that they lead to the same estimate \hat{N} of N and the same asymptotic estimate of $Var(\hat{N})$, so the difference is notable only in higher moments. He further states that 'In fact, if we had to generalize, we could say that the hypergeometric is likely to be appropriate when the main limiting factor on sample size is the trouble involved in marking animals and the multinomial when it is the difficulty in catching them.'. This implies that, for instance, if a population is partly observed by lists of records that contain unique record ID-codes, the multinomial seems to be the most appropriate choice. Finally, Darroch concludes that the multinomial distribution is capable of generalisations that the hypergeometric is unable to accommodate, an advantage that we will use in this paper.

Later, Bishop et al. (1975, p. 446) showed that the assumption of a multinomial distribution can be replaced by

with

$$n_{ab} \sim \operatorname{Poisson}(m_{ab}),$$

$$n_{00} = N - n_{11} - n_{10} - n_{01},$$

without loss of generality. Both the multinomial and Poisson distribution have the practical advantage that they can deal with multiple sources more easily, but the Poisson distribution has a second advantage because it allows the simplification of some derivations due to $\text{Cov}(n_{ab}, n_{\neq ab}) = 0$ and $\text{Cov}(1/n_{ab}, n_{\neq ab}) = 0$.

2.3 Bias reduction in dual-system estimation

Chapman (1951) and Bailey (1951) were the first to be aware of the bias in the LP-estimator. This bias can be easily seen when we assume $n_{ab} \sim \text{Poisson}(m_{ab})$ and write the expectation of the LP-estimator as

$$\mathbf{E}\left[\hat{m}_{00}^{\mathrm{LP}}\right] = \mathbf{E}\left[\frac{n_{10}n_{01}}{n_{11}}\right] = m_{10}m_{01}\mathbf{E}\left[\frac{1}{n_{11}}\right],\tag{7}$$

which is not equal to $\frac{m_{10}m_{01}}{m_{11}}$ because $\mathbb{E}\left[\frac{1}{n_{11}}\right] \neq \frac{1}{m_{11}}$. This shows that under a Poisson distribution, $\frac{1}{n_{11}}$ is the only source of bias in the LP-estimator.

Chapman and Bailey started with the hypergeometric and binomial distribution respectively and used different approximation approaches of the expectation of the ML- estimator to derive their bias-reduced estimators. Bailey used a second-order Taylor series approximation and concludes that

$$\hat{m}_{00}^{\text{Bailey}} = \frac{n_{10}^{\text{Bailey}} n_{01}^{\text{Bailey}}}{n_{11}^{\text{Bailey}}} = \frac{n_{10}(n_{01}-1)}{(n_{11}+1)}$$
(8)

and

$$\hat{N}^{\text{Bailey}} = \frac{n_{1+}(n_{+1}+1)}{(n_{11}+1)}.$$
(9)

are biased reduced estimators for m_{00} and N respectively (Bailey, 1951, p. 295).

Chapman uses a different approach that is recommended by Stephan (1945). Instead of a Taylor approximation, Stephan recommends writing $\mathbf{E}\begin{bmatrix}\frac{1}{x}\end{bmatrix}$, with x a binomial random variable, as a series of inverse factorials, as one needs quite a few terms before a Taylor series becomes reasonably accurate (Stephan, 1945, p. 52). This increased rate of convergence of Stephan's inverse factorial approximation in case of $\mathbf{E}\begin{bmatrix}\frac{1}{x}\end{bmatrix}$ and $n_{11} \sim \text{Poisson}(m_{11})$, is illustrated with a straightforward simulation study presented in Appendix A. Chapman uses Stephan's inverse factorial approximation to derive a bias-reduced expression for $\frac{n_{10}n_{01}}{n_{11}}$ and concludes that a bias-reduced estimator for m_{00} is

$$\hat{m}_{00}^{\text{Chap}} = \frac{n_{10}^{\text{Chap}} n_{01}^{\text{Chap}}}{n_{11}^{\text{Chap}}} = \frac{n_{10} n_{01}}{(n_{11} + 1)},\tag{10}$$

and for N

$$\hat{N}^{\text{Chap}} = \frac{(n_{1+}+1)(n_{+1}+1)}{(n_{11}+1)} - 1.$$
(11)

A Bailey and Chapman estimate can also be obtained from the log-linear model in Eq. (5), if instead of $\mathbf{n}^{\text{LP}} = (n_{11}, n_{01}, n_{01})^{\top}$, respectively, $\mathbf{n}^{\text{Bailey}} = (n_{11} + 1, n_{01}, n_{01} - 1)^{\top}$ and $\mathbf{n}^{\text{Chap}} = (n_{11} + 1, n_{01}, n_{01})^{\top}$ are used.

The Chapman- and Bailey-estimator differ only slightly, but the Chapman-estimator became the standard bias-reduced estimator in DSE literature. A reason could be that Chapman (1951, p. 146) further shows that if $\frac{n_1+n_{+1}}{N} > \log(\frac{N}{\epsilon})$ holds,

$$\left|\mathbb{E}\left[\hat{N}^{\text{Chap}}\right] - N\right| < \frac{\epsilon}{100}N,$$

with ϵ some arbitrary small positive number (Cramer, 1922, p. 502) also holds. This means that if the two sources are large enough compared to N, the bias in \hat{N}^{Chap} is less than ϵ percent of N and so Chapman refers to his estimator as 'essentially unbiased'. Therefore we refer to the Chapman-estimator not only as a bias-reduced, but also as a bias-*corrected* estimator. Chapman, (1951, p. 146) finally notes that the Chapman-estimator requires

$$\frac{n_{1+}n_{+1}}{N} > \log N,\tag{12}$$

to hold. This inequality is derived from setting $\left|\mathbf{E}\left[\hat{N}^{\text{Chap}}\right] - N\right| \leq 1$ and can be considered a regularity condition for the Chapman-estimator. If this regularity condition is not

met, \hat{N}^{Chap} may suffer from considerable (negative) bias, as we will illustrate later in the simulation study in Table 1.

Chapman derived his estimator for the hypergeometric distribution, but it can also be approximated with a second-order Taylor approximation for the multinomial and Poisson distribution, which is derived in Appendix B. This derivation suggests that the Chapmanestimator is also valid under a multinomial or Poisson distribution. This is useful when we extend the Chapman-estimator to multiple sources in Section 3.2. Combining the Chapman-estimator with the results in Appendix A and B imply that if $n_{ab} \sim \text{Poisson}(m_{ab})$ we can write

$$\frac{1}{m_{ab}} \approx \mathbf{E} \left[\frac{1}{n_{ab} + 1} \right]. \tag{13}$$

This equation will allow us to easily extend the Chapman MSE-estimator towards multiple sources in Section 3.2.

Bailey did not extend his estimator to more than two sources. Chapman (1952) did, but he only considered the case where a unit was tagged in an earlier source or not, and did not consider dependence between pairs of sources. Dependence between sources is further discussed in Section 3.1. Others, like Cordeiro and McCullagh (1991), Firth (1993), Evans and Bonett (1994), Rivest and Lévesque (2001), Kosmidis et al. (2020), have proposed bias-reduced estimators for log-linear models in general and therefore do take dependence between sources into account. These models are discussed in more detail in Section 3.1.1. However, we will include these bias-reduced estimators in the simple DSE simulation study presented in Section 2.4.

2.4 Dual-system estimation simulation study

In this section we compare the LP-, Bailey-, Cordeiro, Firth-, Kosmidis, Evans and Bonette (EB)-, Rivest and Lévesque (RL)- and Chapman-estimator in a DSE setting. The LP-, Baileyand Chapman-estimator can only be used in DSE and were discussed in the previous sections. The Cordeiro, Firth-, Kosmidis, EB- and RL-estimator can be applied in both DSE and MSE and will be discussed in Section 3.1.1. We use a Monte Carlo simulation study to compare the different estimators. The method we use to generate contingency tables is discussed in Hammond, van der Heijden, and Smith (2023). It allows us to start with a log-linear model having prespecified inclusion probabilities p_A and p_B and odds ratio(s) and generate contingency tables from this model. The resulting n_{ab} are generated from a multinomial distribution. This is particularly useful in the next section in which we consider more than two sources, and pairs of sources that are dependent.

A minor but important simulation issue is the regularity condition in Eq. (12), or the issue of what (Otis, Burnham, White, & Anderson, 1978, p. 125) refer to as 'failures'. This implies that the relation between n_{1+} , n_{+1} and N must be set such that they comply to Eq. (12). A simple example of a failure is when, in DSE, n_{11} equals zero, which leads to $\hat{N}^{\text{LP}} = \infty$. Otis et al. (1978) recommend replacing such a replication with a new replica-

tion, an advice that was followed in Evans and Bonett (1994). However, replacing failure replications, that correspond to large population size estimates, with new population size estimates, introduces selection bias in the sense that, when \hat{N}^{est} is an unbiased estimator for N, the mean of these estimates \bar{N}^{est} departs from N. Therefore, to obtain accurate mean estimates that allow a fair comparison of bias between the different estimators, we choose the combined N, p_A and p_B such that for scenario 1 - 6 the probability of failures becomes close to zero. Nonetheless a failure occurred once for scenario 1. These settings also imply that the regularity condition in Eq. (12) holds by a substantial margin.

The scenario parameters are shown in the columns N, p_A and p_B of Table 1 below. Scenarios 1 - 6 comply to Chapman's regularity condition in Eq. (12). To see how estimators are affected when this regularity condition is violated, we have added a 7th scenario under which the regularity condition does not hold, i.e. $n_{1+} = n_{+1} = 15$, so $n_{1+}n_{+1}/N = 225/100 < \log 100$. The different estimators that are compared are shown in the columns that follow. In the context of DSE some estimators are equivalent and their results are displayed in a single column. This holds for \hat{N}^{EB} , $\hat{N}^{\text{Cordeiro}}$, \hat{N}^{Firth} and $\hat{N}^{\text{Kosmidis}}$ (denoted as $\hat{N}^{\text{EB/CFK}}$), and for \hat{N}^{Chap} and \hat{N}^{RL} (denoted as $\hat{N}^{\text{Chap/RL}}$).

S	N	p_A	p_B	\bar{n}	$ar{N}^{ ext{LP}}$	$ar{N}^{Bailey}$	$ar{N}^{ ext{EB/CFK}}$	$ar{N}^{ extsf{Chap}/ extsf{RL}}$
1	100	0.5	0.2	60.0	105.3***†	96.1***	105.2***	100.1
2	100	0.35	0.3	54.5	106.0***	98.0***	105.3***	100.4^{*}
3	500	0.4	0.15	244.9	508.3***	493.6***	507.4***	499.2
4	500	0.25	0.2	200.1	512.4***	495.4***	509.3***	499.4
5	10,000	0.3	0.1	3,699.2	10,018.0***	9,987.9***	10,013.1***	9 <i>,</i> 996.9
6	10,000	0.25	0.15	3,624.9	10,016.7***	9 <i>,</i> 993.9*	10,012.5***	9,999.6
7	100	0.15	0.15	27.8	$146.2^{***\dagger}$	87.2***	128.0***	92.3***

Table 1: Simulation study with 20,000 replications for seven DSE scenarios.

 \bar{n} gives the mean number of observed units n over all replications. The superscripts *, ** and *** indicate that we can reject $\hat{N}^{\text{est}} = N$ with a two-sided t-test with p-values = 0.05, 0.01 and 0.001 respectively. A \dagger as superscript indicates that extremely high estimates due to failures were replaced with the highest Chapman estimate in the simulation sample.

The *s in the column of $\hat{N}^{\text{Chap/RL}}$ indicate that for p-value = 0.05, in five out of the six regular scenarios, the hypothesis $N = \hat{N}^{\text{Chap/RL}}$ cannot be rejected. For p-value = 0.01 this holds for all six regular scenarios. The same does not hold for the other estimators, for which the mean over all replications, in most cases, significantly differs from N for p-value = 0.001, and for all cases for p-value = 0.05. For all scenarios the bias in $\hat{N}^{\text{Chap/RL}}$ is smaller than the bias in the other estimators. This shows that in DSE, the Chapman- and RL-estimator are superior to the other estimators. If Chapman's regularity condition in Eq. (12) is not met, as in scenario 7, all estimators are considerably biased.

The standard deviation(SD) and root mean squared errors (RMSEs) that correspond to each estimator and scenario in Table 1 can be found in Table C1 in Appendix C.1. This table shows that the SDs and RMSEs of the Bailey- and Chapman/RL-estimator are smaller than the RMSEs of the EB/CFK-estimator, which in turn are smaller than the RMSEs of the ML-estimator.

3 Multiple-systems estimation

This section discusses multiple-systems estimation (MSE). First it introduces some notation additional to the DSE notation introduced in Section 2. Next, Section 3.1 proceeds with some MSE preliminaries and bias-reduced MSE estimators. In Section 3.2 we derive a new bias-corrected estimator that can be considered an extension of the Chapman-estimator towards MSE under saturated models. In Section 3.3 the Chapman MSE-estimator is further generalised towards all log-linear models, both saturated and restricted.

MSE considers the case where a population that consists of N unique units is partly observed by a set of k sources, indicated by A, B, C, \ldots . For ease of notation we will, where possible, discuss MSE from the perspective of three sources, because it can often be generalised to k sources in a straightforward way. For three sources, the inclusion pattern is denoted as abc with a, b, c = 1, 0, with the same meaning as ab in DSE notation. For ksources the inclusion pattern is $ab \dots k$. We introduce notation that allows us to distinguish between the sets of unit counts that are observed an *even* and *odd* number of times, that we denote by n_{even} (or $m_{\text{even}}, \hat{m}_{\text{even}}$) and n_{odd} (or $m_{\text{odd}}, \hat{m}_{\text{odd}}$). For three sources this gives $n_{\text{odd}} = (n_{111}, n_{100}, n_{010}, n_{001})$ and $n_{\text{even}} = (n_{110}, n_{101}, n_{011})$.

In contrast to DSE, in MSE the log-linear model can take different forms. Therefore, the superscript in \hat{N}^{est} , n_{ab}^{est} and $\hat{m}_{ab}^{\text{est}}$ is extended to $\hat{N}^{\text{est,LLM}}$, $n_{abc}^{\text{est,LLM}}$ and $\hat{m}_{abc}^{\text{est,LLM}}$, where 'est,LLM' specifies not only the chosen estimator but also the chosen log-linear model.

3.1 Preliminaries

The first to consider more than two sources was Schnabel (1938). After this the use of multiple sources became more common and estimators were introduced that made use of different distributional assumptions. For instance, Chapman (1954), Darroch (1958) and Cormack and Jupp (1991) assumed every element in n_{abc} to be an independent realisation from a Poisson distribution. This is a reasonable assumption when n_{abc} are relatively small compared to N, but when this is not true, one should take into account that each m_{abc} has an upper-bound of N. Adding this restriction to the Poisson distribution assumption is equivalent to assuming that the joint set of n_{abc} has a multinomial distribution with expectations m_{abc} for which $m_{000} + \sum_{abc} m_{abc} = N$ (see e.g. Bishop et al., 1975; Darroch, Fienberg, Glonek, & W, 1993; Sanathanan, 1972; Wolter, 1986).

In case of three sources the independence assumption that holds in DSE is relaxed and it is sufficient to assume that two conditional odds-ratios given the levels of the third source are equal. For example, for the two odds-ratios of source *A* and *B* given source *C*

$$\frac{m_{110}/m_{100}}{m_{010}/m_{000}} = \frac{m_{111}/m_{101}}{m_{011}/m_{001}},\tag{14}$$

which gives

$$m_{000} = \frac{m_{111}m_{100}m_{010}m_{001}}{m_{110}m_{101}m_{011}}.$$
(15)

A general expression is provided by Fienberg (1972), who states that for k sources, $m_{00...0}$ can be written as

$$m_{00\dots0} = \frac{\prod m_{\text{odd}}}{\prod m_{\text{even}}}.$$
(16)

For three sources, the saturated (SAT) log-linear model for the seven observed counts becomes

SAT:
$$\log m_{abc} = \lambda + \lambda_a^A + \lambda_b^B + \lambda_c^C + \lambda_{ab}^{AB} + \lambda_{ac}^{AC} + \lambda_{bc}^{BC}$$
, (17)

where the parameters are identified by setting them to zero if one or more of the subscripts are 0. In comparison to DSE, in the saturated log-linear model the independence assumption is replaced by the assumption of no three-factor interaction, i.e $\lambda_{abc}^{ABC} = 0$. The interaction parameters λ_{ab}^{AB} , λ_{ac}^{AC} and λ_{bc}^{BC} allow for interactions between pairs of sources, and thus the model is less restrictive than the DSE model and hence more realistic in applications.

For three sources, the saturated model is not the only log-linear model that can be used. If the parameters of one or more pairs of sources are set to zero (e.g. $\lambda_{ab}^{AB} = 0$), we have a *restricted* log-linear model. An advantage of further restricted models is that the resulting estimates have smaller variance than estimates from less restricted models (Bishop et al., 1975, p. 242). A disadvantage is that they give biased estimates if the assumed restriction does not hold. We discuss restricted models in more detail because, as we will see in Section 3.3, the precise model specification affects the bias-corrected estimator. Fienberg (1972) and Bishop et al. (1975) discuss the three possible alternative log-linear model formulations for three sources where all direct inclusion parameters λ_a , λ_b and λ_c are included. Starting from the saturated log-linear model SAT in Eq. (17), they discuss the two-pair dependence (2PD), the one-pair dependence (1PD), and independence (IND) model. Examples of 2PD and 1PD are

$$2PD: \log m_{abc} = \lambda + \lambda_a^A + \lambda_b^B + \lambda_c^C + \lambda_{ab}^{AB} + \lambda_{bc}^{BC},$$
(18)

$$1PD: \log m_{abc} = \lambda + \lambda_a^A + \lambda_b^B + \lambda_c^C + \lambda_{ab}^{AB}$$
(19)

and

$$IND: \log m_{abc} = \lambda + \lambda_a^A + \lambda_b^B + \lambda_c^C.$$
(20)

It suits our purpose to write these models as in Eq. (5). They all use $\mathbf{n} = \mathbf{n}^{\text{ML}} = (n_{111}, n_{101}, n_{011}, n_{010}, n_{010}, n_{001})$, but differ with respect to $\boldsymbol{\lambda} = \boldsymbol{\lambda}^{\text{LLM}}$ and $\mathbf{X} = \mathbf{X}^{\text{LLM}}$. $\boldsymbol{\lambda}^{\text{LLM}}$ simply consists of the λ 's in the corresponding LLM and \mathbf{X}^{LLM} becomes X_{abc}^{SAT} , X_{abc}^{2PD} , X_{abc}^{1PD} or X_{abc}^{IND} written as

respectively. Estimating one of these models with ML gives the fitted-values $\hat{m}_{abc}^{\text{ML,LLM}}$. A general expression for $m_{000}^{\text{ML,LLM}}$ is obtained by replacing the m_{abc} in Eq. (15) with the ML estimates $\hat{m}_{abc}^{\text{ML,LLM}}$. For LLM = SAT this gives $m_{abc}^{\text{ML,LLM}} = m_{abc}^{\text{ML,SAT}} = n_{abc}$ and thus

$$\hat{m}_{000}^{\text{ML,SAT}} = \frac{n_{111}n_{100}n_{010}n_{001}}{n_{110}n_{101}n_{011}}.$$
(21)

For model 2PD and 1PD Fienberg (1972, p. 596) shows this expression can be further simplified, i.e.,

$$\hat{m}_{000}^{\text{ML,2PD}} = \frac{n_{100}n_{001}}{n_{101}} \tag{22}$$

and

$$\hat{m}_{000}^{\text{ML,1PD}} = \frac{n_{001}n_{++0}}{n_{111} + n_{101} + n_{011}}.$$
(23)

For model IND, such a closed form solution does not exist. However, for IND an estimate can be obtained by replacing the m_{abc} in Eq. (15) with the fitted-values $\hat{m}_{abc}^{\text{ML,IND}}$. (Fienberg, 1972, p. 597) shows that this is in fact an approach that can be generally used, where Eq. (16) gives an estimate of the missing cell for any log-linear model with any number of sources. Note that the LP-estimator in Eq. (3) can be considered a special of (16), with k = 2 and LLM=SAT.

Bias reduction in multiple-systems estimation 3.1.1

MSE is based on a log-linear model estimated with ML, which is well known to give biased estimates (see e.g. Hald, 1952, chap. 7, or Miller, 1984). In this context, an approach to obtain bias-reduced ML estimates is also known as generalized linear models (GLMs) using adjusted score functions (see e.g. Firth, 1993; Kosmidis et al., 2020). A DSE example of this approach can be found in Section 2.3, where replacing n with the adjusted n^{Chap} or n^{Bailey} led to the bias-reduced DSE estimators by Chapman and Bailey. Cordeiro and McCullagh (1991); Firth (1993); Kosmidis and Firth (2011) and others use this approach to obtain biasreduced ML-estimators for generalised linear models, such as the log-linear model, that can also be applied to MSE. In literature we also find bias-reduced MSE estimators that are developed specifically in the context of MSE, such as by Evans and Bonett (1994) and Rivest and Lévesque (2001). However, despite that they are developed in the more specific MSE context, these bias-reduced MSE estimators also fit what Firth (1993) refers to as the more general (GLMs with) modified-score functions approach.

The simplest bias-reduced MSE estimator is proposed by Evans and Bonett (1994), which we denote as $\hat{N}^{\text{EB},\text{LLM}}$. They propose to use the adjusted $\mathbf{n}^{\text{EB}} = \mathbf{n} + 0.5^{(k-1)}$ in (5) instead of \mathbf{n} . This is the result of a compromise between Berkson (1955) and Plackett (1981). In a log-linear regression model, Berkson proposes to replace values in n_{abc} that are equal to zero with $0.5^{(k-1)}$, and Plackett (1981), who states that if $n_{abc} \sim \text{Poisson}(m_{abc})$, then $\log(n_{abc} + 0.5)$ instead of $\log(n_{abc})$ is a more accurate estimate for $\log(m_{abc})$.

Another bias-reduced estimator that was developed specifically for MSE was proposed by Rivest and Lévesque (RL, 2001). They propose a bias reduction method that can be used to reduce bias in a set of MSE estimators proposed by Otis et al. (1978) in the context of wildlife populations. Unfortunately, with the exception of the independence model, which corresponds to the M_t model, the other models by Otis et al. do not correspond exactly to Eq. (17) - (19). For the SAT, 2PD and 1PD model, we consider the adjusted counts that belong to model M_{th} as the most appropriate choice, because it is most similar. See (Evans, Bonett, & McDonald, 1994) for further discussion on this topic. The bias reduction by Rivest and Lévesque is derived from a standard result by McCullagh and Nelder (1989), about the bias in estimators in generalized linear models. McCullagh and Nelder derive an asymptotic bias expression for estimates based on models with canonical link functions, such as the log-linear model. For two sources, the resulting RL-estimator is equal to the Chapman-estimator, as was seen in Table 1. We denote the RL-estimator as $\hat{N}^{\text{RL,LLM}}$ and their adjusted count as $\mathbf{n}^{\text{RL,LLM}}$, with $\mathbf{n}^{\text{RL,ND}} = \mathbf{n}^{\text{RL,M_t}}$ and $\mathbf{n}^{\text{RL,SAT/2PD/1PD}} = \mathbf{n}^{\text{RL,M_{th}}}$. For three sources they become (Rivest & Lévesque, 2001, p. 562):

$$\mathbf{n}^{\mathrm{RL},M_t} = (n_{111}, n_{110} + \frac{1}{3}, n_{101} + \frac{1}{3}, n_{011} + \frac{1}{3}, n_{100} + \frac{1}{6}, n_{010} + \frac{1}{6}, n_{001} + \frac{1}{6})^{\top}$$
(24)

and

$$\mathbf{n}^{\mathrm{RL},M_{th}} = (n_{111}, n_{110} + \frac{1}{3}, n_{101} + \frac{1}{3}, n_{011} + \frac{1}{3}, n_{100}, n_{010}, n_{001})^{\top}.$$
(25)

Rivest and Lévesque (2001) show in a simulation study that their estimator outperforms the EB-estimator in terms of bias reduction.

Bias reduction in MSE by means of the modified-score functions approach (Firth, 1993) relies on the same standard result about the bias of estimators in GLMs by McCullagh and Nelder (1989) as was used by Rivest and Lévesque (2001). It was used by Cordeiro and McCullagh (1991); Firth (1993); Kosmidis (2007); Kosmidis and Firth (2011) and others to reduce bias in parameter estimates in log-linear models. Cordeiro and McCullagh, Firth and Kosmidis and Firth give three different bias-reduced parameter estimates $\hat{\lambda}^{est}$ for the λ in Eq. (5), which correspond to three different bias-reduced estimators $\hat{m}_{000}^{est} = \exp \hat{\lambda}^{est}$. The description of the details on these estimators are beyond the scope of this paper, but they are provided in Kosmidis (2014); Kosmidis and Kenne Pagui (2023); Kosmidis et al. (2020). In this paper we limit ourselves to noting that in the DSE and MSE simulation studies presented in this paper we found negligible differences between them, and therefore we denote them as the single estimator $\hat{N}^{CFK,LLM}$.

In the next section we extend the Chapman-estimator towards multiple sources, which

results in a Chapman MSE-estimator that differs from the estimators discussed in this section, both for the saturated and more restricted log-linear models.

3.2 The Chapman MSE-estimator for saturated models

To derive an Chapman MSE estimator we start with the result of Bishop et al. (1975, p. 446), who showed that the MLEs for m_{abc} are equivalent under the assumption that n_{abc} follows either a Poisson or multinomial distribution, provided that $\sum_{abc} m_{abc} + m_{000} = N$. Combining the implications of the Chapman-estimator as discussed in Section 2.3 with the MSE models discussed in Section 3.1 under the assumption of a Poisson distribution allows us to derive a bias-corrected MSE estimator in a straightforward way. The Poisson distribution implies that $\text{Cov}(n_{abc}, n_{\neq abc}) = 0$ and $\text{Cov}(1/(n_{abc} + 1), n_{\neq abc}) = \text{Cov}(1/n_{abc}, n_{\neq abc}) = 0$, when we combine this with Eq. (13) and (16) this gives

$$m_{00\dots0} = \frac{\prod m_{\text{odd}}}{\prod m_{\text{even}}} \approx \prod \mathbf{E} \left[n_{\text{odd}} \right] \prod \mathbf{E} \left[\frac{1}{(n_{\text{even}} + 1)} \right] = \mathbf{E} \left[\frac{\prod n_{\text{odd}}}{\prod (n_{\text{even}} + 1)} \right],$$
(26)

which suggests

$$\hat{m}_{000}^{\text{Chap MSE,SAT}} = \frac{n_{111}n_{100}n_{010}n_{001}}{(n_{110}+1)(n_{101}+1)(n_{011}+1)}$$
(27)

as a bias-corrected estimator for three sources, and

$$\hat{m}_{00...0}^{\text{Chap MSE,SAT}} = \frac{\prod n_{\text{odd}}}{\prod (n_{\text{even}} + 1)}$$
(28)

for any number of sources.

When we compare the Chapman MSE-estimator in Eq. (27) with the RL-estimator in Eq. (25), it becomes clear that the equality between both estimators in DSE does not hold for MSE. We further note that Chapman MSE estimates can also be obtained with Eq. the Poisson regression model as defined in Eq. (5), by using the modified counts $n_{abc}^{Chap MSE,SAT}$ instead of **n**.

3.2.1 Simulation study with saturated models

In Section 2.4 we have seen that the Chapman- and RL-estimator are equivalent and less biased than the alternative DSE estimators. This equivalence is unlikely to hold in MSE, because they are no longer the same estimators. Here we compare them in a simulation study, together with other bias-reduced MSE estimators. We consider fourteen scenarios. The scenarios in Table 2 differ with respect to the size of the population N, the number of sources k and log-linear model specifications (i.e. different values for p_A , p_B , p_C , p_D , θ^{AB} , θ^{AC} , θ^{AD} , θ^{BC} and θ^{CD} , see Hammond et al., 2023, for further details). The odds-ratios are chosen such that scenario 1 - 3 and 13 concern LLM = IND, scenario 4 - 6 concern LLM = 1PD, scenario 7 - 9 concern LLM = 2PD, scenario 10 - 12 concern LLM = SAT and finally scenario 14 concerns LLM = 4PD (i.e. four pairs of dependent sources). The different parameters are chosen such that the probability of failures in each scenario is small.

S	LLM	$\mid N$	k	p_A	p_B	p_C		θ_{AB}	θ_{AC}	θ_{BC}	
1		100	3	0.5	0.4	0.3		1	1	1	
2	IND	500	3	0.4	0.3	0.2		1	1	1	
3		10,000	3	0.35	0.3	0.25		1	1	1	
4		100	3	0.5	0.4	0.3		1.5	1	1	
5	1PD	500	3	0.4	0.3	0.2		1.5	1	1	
6		10,000	3	0.35	0.3	0.25		1.5	1	1	
7		100	3	0.5	0.4	0.3		1.5	1	0.5	
8	2PD	500	3	0.4	0.3	0.2		1.5	1	0.5	
9		10,000	3	0.35	0.3	0.25		1.5	1	0.5	
10		100	3	0.5	0.4	0.3		1.5	0.75	0.5	
11	SAT	500	3	0.4	0.3	0.2		1.5	0.75	0.5	
12		10,000	3	0.35	0.3	0.25		1.5	0.75	0.5	
S	LLM	N	k	p_A	p_B	p_C	p_D	θ_{AB}	θ_{AD}	θ_{BC}	θ_{CD}
13	IND	20,000	4	0.4	0.35	0.3	0.25	1	1	1	1
14	4PD	20,000	4	0.4	0.35	0.3	0.25	1.5	1.5	0.75	0.5

Table 2: MSE simulation scenarios

The estimates presented in Table 3 are based on the assumption of a saturated model. This means that for all scenarios, except scenario 10 - 12, the model is overspecified. Overspecification only affects the variance and not the mean of an estimator, so it does not lead to the introduction of bias, although it may increase the bias when it is present. In contrast to the DSE simulation study in Section 2.4, it was not possible to exclude failures in all scenarios, in particularly for N = 100. In those cases the failures where replaced with the highest value of all Chapman MSE-estimators for that scenario, indicated by a superscript \dagger in the cell.

The results in Table 3 indicate that, given an assumed saturated model, the Chapman MSE-estimator performs best of the tested estimators, irrespective of the underlying LLM. For p = 0.01 it gives a mean value that cannot be rejected to be different from N in 13 out of 14 scenarios. Also, in the scenarios where the Chapman MSE-estimator shows some statistically significant bias (S = 4, 7 and 10), the bias is small in itself and much smaller than in the other estimators. For the IND and 1PD model with large N, the bias of the ML, EB and CFK-estimators is equally large. This unexpected indifference might be due to the modification of elements of n_{abc} that are in the numerator of the ML-estimator, which, as we have seen in Section 3.2, is unnecessary. The RL-estimator performs clearly better than the EB- and CFK-estimator, but still shows some statistically significant bias for most scenarios, especially when N = 100 or 500.

The SEs and RMSEs that correspond to each estimator and scenario in Table 3 can be found in Table C2 and C3 in Appendix C.2. These tables show that under an assumed saturated model, the Chapman estimator not only outperforms the other estimators in

\overline{S}	N	\bar{n}	$ar{\hat{N}}^{ ext{ML,SAT}}$	$ar{N}^{ ext{EB}, ext{SAT}}$	$\bar{\hat{N}}$ CFK,SAT	$ar{\hat{N}}^{ extsf{RL}, extsf{SAT}}$	$\hat{\hat{N}}$ Chap MSE,SAT
1	100	79.0	112.7***†	112.4***	110.9***	103.3***	100.1
2	500	332.0	520.8***	521.1***	521.3***	506.1***	499.3
3	10,000	6,587.7	10,015.5***	10,016.3***	10,017.1***	10,004.1	9 <i>,</i> 998.5
4	100	77.3	115.3***†	114.4***	111.7***	103.4***	99.6*
5	500	323.8	525.2***	524.4***	523.8***	508.3***	500.7
6	10,000	6,439.5	10,015.7***	10,016.0***	10,016.2***	10,003.5	9,997.4
7	100	79.1	121.5***†	119.0***	113.2***	103.8***	99.5**
8	500	330.3	532.1***	530.7***	529.4***	509.9***	500.4
9	10,000	6,608.9	10,019.6***	10,020.4***	10,021.1***	10,006.1*	9,999.3
10	100	80.0	117.8***†	115.6***	111.9***	103.2***	99.4***
11	500	334.1	529.7*** [†]	529.9***	529.6***	509.3***	500.4
12	10,000	6,690.3	10,019.6***	10,020.9***	10,022.3***	10,006.4*	9,999.8
13	20,000	15,905.3	20,051.8***	20,051.7***	20,051.6***	20,043.5***	20,004.1
14	20,000	15,834.5	20,049.4***	20,050.2***	20,052.6***	20,039.9***	19,992.4

Table 3: Simulation study with assumed saturated log-linear models, with 20,000 replications for MSE scenarios 1 - 14, for MSE scenario 1 - 14 in Table 2.

 \bar{n} gives the mean number of observed units n over all replications. The superscripts *, ** and *** indicate that we can reject $\hat{N}^{\text{est}} = N$ with a two-sided t-test with p-values = 0.05, 0.01 and 0.001 respectively. A \dagger as superscript indicates that extremely high estimates due to failures were replaced with the highest Chapman MSE estimate in the simulation sample.

terms of bias, but also in terms of SD and RMSE, in particular for smaller N, irrespective of the true model as given in the column LLM.

The estimates in Table 3 are based on the saturated model, but more restricted models such as those in Eq. (18), (19) and (20) might be assumed. In the next section we will therefore discuss the Chapman MSE-estimator for restricted models.

3.3 A generalisation of the Chapman MSE-estimator

The Chapman MSE-estimator for saturated models, as discussed in the previous section, is not necessarily a correct bias-corrected estimator for restricted log-linear models. As an example where the use of the Chapman MSE-estimator for saturated models leads to an incorrect result, consider the 1PD model (19) with estimator (23). When this estimator uses the modified count vector $\mathbf{n}^{\text{Chap MSE, SAT}} = (n_{111}, n_{110} + 1, n_{101} + 1, n_{011} + 1, n_{100}, n_{010}, n_{001})$ instead of the observed count vector \mathbf{n} , this gives

$$\hat{m}_{000}^{\text{Chap MSE',1PD}} = \frac{n_{001}(n_{++0}+1)}{n_{111} + (n_{101}+1) + (n_{011}+1)}.$$

We know that this estimator is not correcting for bias correctly, because the ML-estimator for the 1PD model has the same structure as the LP-estimator, namely the product of two Poisson variables in the nominator (i.e. $n_{001}n_{++0}$) and a single Poisson variable in the denominator (i.e. the sum $n_{111} + n_{101} + n_{011}$). Therefore we should use the same bias-

correction as used in the Chapman-estimator, namely

$$\hat{m}_{000}^{\text{Chap MSE,1PD}} = \frac{n_{001}n_{++0}}{n_{111} + n_{101} + n_{011} + 1}.$$
(29)

This is the correct bias-corrected estimator for the 1PD model. Similarly, for the 2PD model (18) with estimator (22) we have the bias-corrected estimator

$$\hat{m}_{000}^{\text{Chap MSE,2PD}} = \frac{n_{001}n_{100}}{n_{101} + 1}.$$
(30)

For the independence model for three sources, a direct solution for the estimator does not exist and therefore we cannot use the approach adopted for the 1PD and 2PD model as a general solution. Furthermore, for log-linear models with more sources and more source dependencies, the derivations performed by Bishop et al. (1975) become increasingly complex.

Generally, in order to correct for bias, it appears that we should only know which (functions of) observed counts n_{abc} are in the denominator of $\hat{m}_{000}^{\text{ML,LLM}}$, and subsequently adjust these counts to correct for bias. To identify these (functions of) observed counts n_{abc} , we propose to use the Moore-Penrose inverse (MPI, Moore, 1920; Penrose, 1955), that can be used to obtain a 'best fit' (i.e. least squares) solution (if any exists) for systems of linear equations.

3.3.1 Bias reduction by using the Moore-Penrose inverse

We start with the log-linear model in Eq. (5), $\log \mathbb{E}[\mathbf{n}|\mathbf{X}] = \mathbf{X}\lambda$, which is a system of linear equations. A solution for λ can be found with the help of the MPI that we write as $\mathbf{Z} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}$, i.e.:

$$\boldsymbol{\lambda}^{\text{MPI}} = \mathbf{Z} \log \left[\mathbf{n} | \mathbf{X} \right] = \mathbf{Z} \log \mathbf{m}.$$
(31)

For two sources this gives $\mathbf{m} = (m_{11}, m_{10}, m_{01})^{\top}$, $\boldsymbol{\lambda}^{\text{MPI}} = (\boldsymbol{\lambda}^{\text{MPI}}, \boldsymbol{\lambda}^{A, \text{MPI}}_{a}, \boldsymbol{\lambda}^{B, \text{MPI}}_{b})^{\top}$, $\mathbf{X} = X_{ab} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$ and $\mathbf{Z} = \mathbf{Z}_{ab} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{pmatrix}$. We are interested in a solution for

 m_{00} , which is $m_{00} = \exp \lambda^{\text{MPI}}$, and because λ^{MPI} depends only on the first row of \mathbf{Z}_{ab} , only this row is relevant for our purpose. We write this row as the vector $\mathbf{z} = (z_{11}, z_{10}, z_{01})^{\top} = (-1, 1, 1)^{\top}$. Thus (31) allows us to write m_{00} as a function of z_{ab} and m_{ab} , i.e.

$$m_{00} = \exp \lambda^{\text{MPI}} = \exp \sum_{ab} z_{ab} \log m_{ab} = \prod_{ab} (m_{ab})^{z_{ab}} = \frac{m_{10}m_{01}}{m_{11}},$$

which corresponds to Eq. (2) that led to the LP-estimator, so for two sources $\lambda^{\text{MPI}} = \lambda^{\text{ML}}$. However, for our purpose a more important point is that the first element z_{11} in \mathbf{z} has a negative sign, which indicates that m_{11} is in the denominator of the expression for m_{00} . We have seen in Eq. (26), that in order to correct for bias it is important to identify which elements of n are in the denominator.

This relation between z_{ab} and the LP-estimator also holds for z_{abc} and the SAT, 2PD and 1PD ML-estimators, as defined in Eq. (21), (22) and (23). This can be seen when we specify

$$m_{000}^{\text{MPI,LLM}} = \prod_{abc} (m_{abc})^{z_{abc}^{\text{LLM}}}$$

where z_{abc}^{LLM} depends on the design matrices for restricted log-linear models X_{abc}^{LLM} as defined below Eq. (20). For the models SAT, 2PD, 1PD and IND, the vector \mathbf{z}^{LLM} is given in Table 4a.

Table 4	a				Table 4	b			
m	$ \mathbf{z}^{SAT}$	$\mathbf{z}^{2\text{PD}}$	$\mathbf{z}^{1\text{PD}}$	\mathbf{z}^{IND}	m	$ \mathbf{z}_{<0}^{\text{SAT}} $	$\mathbf{z}_{<0}^{\mathrm{2PD}}$	$\mathbf{z}_{<0}^{\mathrm{1PD}}$	$\mathbf{z}_{<0}^{\text{IND}}$
m_{111}	1	0	-1/3	-1/2	m_{111}	0	0	-1/3	-1/2
m_{110}	-1	0	1/3	0	m_{110}	-1	0	0	0
m_{101}	-1	-1	-1/3	0	m_{101}	-1	-1	-1/3	0
m_{011}	-1	0	-1/3	0	m_{011}	-1	0	-1/3	0
m_{100}	1	1	1/3	1/2	m_{100}	0	0	0	0
m_{010}	1	0	1/3	1/2	m_{010}	0	0	0	0
m_{001}	1	1	1	1/2	m_{001}	0	0	0	0

Table 4: The value of \mathbf{z}^{LLM} and $\mathbf{z}^{\text{LLM}}_{<0}$ for each LLM.

Table 4a shows the positive and negative signs in the elements z^{LLM} that correspond to the counts n_{abc} in the numerator and denominator in the SAT, 2PD and 1PD ML-estimators in Eq. (21), (22) and (23). It is useful to define $z_{<0}^{LLM}$, which is a vector equal to z_{abc}^{LLM} for $z_{abc}^{LLM} < 0$, and zero otherwise. $z_{<0}^{LLM}$ is shown in Table 4b for the SAT, 2PD, 1PD and IND model.

For the 2PD and 1PD model the relation between the MPI expression for m_{000} and the ML-estimator is more intricate. For the 1PD model the MPI expression for m_{000} is

$$m_{000}^{\text{MPI,1PD}} = \frac{m_{001} \left(m_{110} m_{100} m_{010} \right)^{\frac{1}{3}}}{\left(m_{111} m_{101} m_{011} \right)^{\frac{1}{3}}}$$

and the ML-estimator in Eq. (23) can also be written as

$$\hat{m}_{000}^{\text{ML,1PD}} = \frac{n_{001} \left(m_{110} + m_{100} + m_{010} \right) / 3}{\left(m_{111} + m_{101} + m_{011} \right) / 3}$$

The MPI expression for m_{000} is a fraction with geometric means of sets of m_{abc} , both in the numerator and the denominator, while the ML-estimator is a corresponding fraction of arithmetic means of n_{abc} . The same relation can be shown for the SAT and 2PD model. Because a sum of Poisson variables is itself a Poisson variable, and Eq. (13) shows that we should add 1 to a Poisson variable in the denominator, where $\mathbf{z}_{<0}^{\text{LLM}}$ provides a distribution of this +1. To illustrate this, in the bias-corrected estimator for the 1PD model in Eq. (29),

1 is added to the sum of the three Poisson variables n_{111} , n_{101} and n_{011} . The same result is obtained by subtracting -1/3 from each of them, which corresponds to subtracting $\mathbf{z}_{<0}^{\text{LLM}}$ from **n**. Thus we have a simple formula that can be used to obtain the Chapman-estimator in Eq. (10) and the bias-corrected estimators in Eq. (21), (29) and (30), i.e.:

$$\mathbf{n}^{\text{Chap MSE, LLM}} = \mathbf{n} - \mathbf{z}_{<0}^{\text{LLM}}$$
(32)

For the IND model Eq. (32) implies we should replace n_{111} with $n_{111} + 1/2$ to obtain a bias-corrected estimator. We cannot compare this result with a closed form expression of the ML-estimator for the IND model, but an intuitive explanation for this adjustment is that if in the denominator there is a Poisson variable multiplied by a 1/2 as is suggested by the MPI expression, we should add 1 multiplied by a 1/2 to correct for bias as well.

Concluding, in Eq. (32) we propose an adjustment that is based on the MPI and can be used for any log-linear model with any number of sources. We have shown for some examples (i.e., for two sources, and for three sources for the models SAT, 2PD and 1PD) that this adjustment works in these instances. The adjustment also works for the saturated model for any number of sources. We provide no proof for other models, such as the model IND for three sources for which no closed form solutions of ML-estimators exist, and restricted models for four or more sources. In the simulation study in the next section we show that also for these models our procedure reduces the bias to a large extend. Finally, we note that the Chapman MSE adjustment of n_{abc} depends on both the log-linear model and the exact inclusion pattern abc, which is more extensive than the information other estimators use.

3.3.2 Multiple-systems estimation simulation study with restricted models

In Table 5 below we show the result of a simulation study in which we test the Chapman MSE estimators under the different scenarios presented in Table 2, and compare them with the other estimators described in Section 3.1.1. The number of replications is increased from 20,000 to 60,000, because in comparison to Table 3, the estimates are much more accurate because they are based on the same log-linear model that underlies the generation of the contingency table. This is indicated by the LLM⁺ in the subscript. Scenarios 10 - 12 are removed because they represent scenarios in which the saturated model is the true model, and therefore the results of these scenarios are already provided in Table 3. The increase of accuracy implies that, compared to the simulation study presented in Section 3.2.1, more replications are required to statistically reject unbiasedness in estimators with a t-test.

Table 5 shows that if the correct log-linear model is used to estimate N, all estimators have less bias than under the saturated model as presented in Table 3. This is unsurprising, because for the presented scenarios the model that is used for estimation is less overspecified than the saturated model that was used for Table 3. For S = 13, the bias is statistically insignificant in all estimators. The size of the bias in the ML-, EB- and CFK-estimator is

S	N	\bar{n}	$\hat{N}^{\mathrm{ML,LLM^+}}$	$\hat{N}^{ ext{EB,LLM}^+}$	$\hat{N}^{\mathrm{CFK,LLM^{+}}}$	$\hat{N}^{ ext{RL,LLM}^+}$	$\hat{\hat{N}}$ Chap MSE,LLM $^+$
1	100	79.0	100.5***	100.7***	100.9***	100.7***	99.9***
2	500	332.0	501.5***	501.1***	501.9***	501.3***	499.9
3	10,000	6,587.3	10,001.0*	10,000.6	10,001.4**	10,000.8	9,999.4
4	100	77.3	101.2***	101.3***	102.1***	99.9	100.0
5	500	323.8	503.5***	502.6***	504.2***	499.6*	500.2
6	10,000	6,439.6	10,003.1***	10,002.5***	10,003.7***	10,000.1	10,000.4
7	100	79.1	102.7***†	102.8***	102.8***	100.8***	99.9
8	500	330.3	505.9***	505.6***	505.3***	501.7***	499.8
9	10,000	6,608.9	10,005.0***	10,004.8***	10,004.7***	10,001.5	9,999.7
13	20,000	15,320.0	20,000.3	19,999.9	20,000.7	20,000.3	19,999.4
14	20,000	15,166.8	20,002.4***	20,002.3**	20,002.4***	20,001.4*	20,000.5

Table 5: Simulation study with correctly specified log-linear models, with 60,000 replications, for MSE scenario 1 - 9, 13 and 14 in Table 2.

 \bar{n} gives the mean number of observed units n over all replications. The superscript ⁺ indicates that the estimates are obtained under the correctly specified log-linear model, as given in the 'LLM' column in Table 2. The superscripts *, ** and *** indicate that we can reject $\hat{N}^{\text{est}} = N$ with a two-sided t-test for p-values = 0.05, 0.01 and 0.001 respectively. A [†] as superscript indicates that extremely high estimates due to failures were replaced with the highest Chapman MSE estimate in the simulation sample.

comparable and small, and the RL-estimator has less bias than these three estimators. The Chapman MSE-estimator is the only estimator for which unbiasedness cannot be statistically rejected in all except for one scenario. Only in S = 1 there is some statistically significant bias, but this bias is small in itself and less than the bias in the other estimators. To conclude, also when the correct (restricted) model is used to estimate N, the Chapman MSE-estimators outperforms the other estimators, although for simpler models the impact becomes less substantial because the bias is smaller in the first place.

The substantial difference in the magnitude of the bias shown in Tables 3 and 5, is caused by the inflationary effect of variance on positive bias in log-linear models. Less restricted models have larger variance (Bishop et al., 1975, p. 242) and its inflationary effect on the bias can be seen when the bias is written as $\bar{m}_{000}^{\text{est}} - m_{000} = \overline{\exp \hat{\lambda}^{\text{est}}} - \exp \lambda$, where given some positive bias in $\hat{\lambda}^{\text{est}}$, a larger variance in $\hat{\lambda}^{\text{est}}$ leads to a further increase of $\overline{\exp \hat{\lambda}^{\text{est}}}$ and therefore the bias.

Particularly interesting are scenarios for which we were not able to prove mathematically that our MPI procedure is correct, i.e. 1, 2, 3, 13 and 14, as these are scenarios in which the independence model and/or four sources are used. In these scenarios the Chapman MSE-estimator provides estimates with clearly less bias than the bias in the other estimators, and also little bias in general. This is support for the approach that we adopted for the development of the bias-reduced estimators based on Eq. (32).

The SDs and RMSEs that correspond to each estimator and scenario in Table 5 can be found in Table C4 and C5 in Appendix C.3. These tables show that, just like the bias, also the SD and RMSE are smaller when the correctly specified log-linear model is used

for estimation. Also in this case, the RL- and Chapman MSE-estimator outperform the other estimators, especially for models with more parameters. Similar to bias, for the 2PD and SAT model (for SAT see Table 3, C2 and C3) we see that the Chapman MSE-estimator outperforms the RL-estimator in terms of SD and RMSE. This shows that the correction for bias becomes more important when the estimated model has more parameters.

Finally, we note that the Chapman MSE-estimator suffers less from adding irrelevant variables to the model. To illustrate this we consider scenario S = 7 from Table 2, for which the saturated model contains the irrelevant parameter λ_{ac}^{AC} . When we consider the SDs of the Chapman MSE-estimator for this scenario, as shown in Table C2 and C4, we see that it approximately doubles from 12.3 to 24.7. For the other estimators adding the irrelevant parameter λ_{ac}^{AC} has a larger impact on the SD, as it increases approximately three to six times while starting from approximately the same level. The same relation holds for the RMSE.

4 Example: Number of homeless people in the Netherlands

A population size estimate of the homeless people in the Netherlands is published annually by Statistics Netherlands. This estimate is an ML estimate that is based on a MSE model that is discussed in detail in Coumans, Cruyff, Van der Heijden, Wolf, and Schmeets (2017). The estimate is based on a log-linear model that contains three sources and several (categorical) covariates, such as gender (g, 2 categories), age (a, 3 categories), place of living, in- or outside one of the big four Dutch cities (p, 2 categories) and region of origin (o, 3 categories). Together there are 36 subgroups that have observed frequencies denoted as n_{gapo} and an observed frequency with a specific inclusion pattern denoted as $n_{abc,gapo}$. Which sources, covariates and interactions between them are included in the log-linear model, is the result of an Akaike information criterion (AIC) based model selection procedure that is explained in Coumans et al. (2017). Recent work by Silverman (2020) suggests that other model selection approaches based on Bayesian approaches could lead to more robust and stable results, but this is beyond the scope of this paper.

In this practical example, for the years 2009 - 2018, 2020 and 2021, we replicate the model selection and estimation procedure as explained in Coumans et al. (2017). Data for 2019 is unavailable. This gives a series of annual ML estimates for the population size of homeless people in The Netherlands. For each year, the log-linear model that was used to calculate the ML estimate is also used to calculate the corresponding Chapman MSE estimate. This allows us to calculate the difference between the ML and Chapman MSE estimates, all other factors held constant, in a practical example.

In Figures 1a-c below we show, respectively, the original ML estimates and the Chapman MSE estimates of the total number of homeless people, the total number of homeless men and the total number of homeless women, including their two-sided 95% confidence intervals. Note that each figure has its own scale on the y-axis. Figure 1: Total number of homeless people, homeless men and homeless women in the Netherlands over the period 2009-2018 and 2020-2021.





Figure 1a shows ML and Chapman MSE estimates of the total number of homeless people over time, together with their confidence intervals. The ML estimates are between a minimum of 9.5% and a maximum of 25.5% larger than the Chapman MSE-estimator. The confidence interval of the Chapman MSE-estimators is clearly smaller. Figure 1b and 1c show that the total annual difference between both estimators, as was observed in Figure 1a, is not proportionally divided over men and women. In fact, the Chapman MSE-estimator has, relatively, a much larger impact on the estimate of the number of homeless women, which is the smaller group. For women the difference between the estimates is between a minimum of 19.5% in 2017 and a maximum of 51.2% in 2018.

In this practical application the impact of using the Chapman MSE-estimator instead of the ML-estimator is larger than the impact we have seen in the simulation studies. The reason for this difference is twofold. First, the scenarios in the simulation studies were set such that the probability of estimation failures was very small, which led to a mean coverage (i.e. \bar{n}/N) that was large compared to the coverage in our example of homeless people. Second, the MSE model to estimate the number of homeless people involves the use of (categorical) covariates to control for heterogeneity in inclusion probabilities. Because for some homeless people their background characteristics are missing, the estimation procedure uses an expectation–maximization (EM) algorithm to impute missing data (see Coumans et al., 2017, for further details), which for some inclusion patterns may lead to observed frequencies between zero and one. To see why this is important we zoom in on the underlying subgroup estimates for men and women in the year 2021 presented in Table 6 below.

Table 6 presents 18 subgroups indicated by G_{apo} for both men and women. For each subgroup we show both the total observed count n_{gapo} and the observed count $n_{101,gapo}$ for inclusion pattern 101. This specific inclusion pattern is shown because the selected log-linear model is a 2-pair dependence model, for which Table 4 tells us that $n_{101}^{\text{Chap}} = n_{101} + 1$ is the only adjusted observed frequency, while the other elements in n_{abc}^{Chap} are equal to n_{abc} . The difference between $n_{101,gapo}$ and $n_{101,gapo}^{\text{Chap}}$ should therefore explain the difference between N_{gapo}^{Chap} . This difference is shown in the columns $\Delta_{Mapo}^{\text{Chap-ML}}$ and $\Delta_{Wapo}^{\text{Chap-ML}}$.

When we compare the columns $\Delta_{Mapo}^{\text{Chap-ML}}$ and $\Delta_{Wapo}^{\text{Chap-ML}}$ in Table 6, we see that despite the fact that observed counts of men are larger than those of women, differences in counts of subgroups of men and women are very similar. This can be explained by the smaller observed frequencies for women with inclusion pattern 101, that are sometimes even between zero and one, as can be seen in the columns of $n_{101,Mapo}$ and $n_{101,Wapo}$. Adding 1 to such a small number has a relatively large impact on the population size estimate.

Finally, we note that the Chapman MSE estimates follow a similar trend as the MLestimates, which is relevant in practice. Only for the period 2018 - 2020, where the MLestimate is a decrease while the Chapman MSE-estimate is an increase. This might be due to the large ML-estimate in 2018. Furthermore, the estimates and conclusions presented in this section should be treated with some care because for the log-linear model that was used, a regularity condition such as the one for DSE given by Chapman in Eq (12) may

			Men					Women		
G_{apo}	n_{Mapo}	$n_{101,Mapo}$	$\hat{N}_{Mapo}^{\rm ML}$	\hat{N}_{Mapo}^{Chap}	$\Delta^{\rm Chap-ML}_{Mapo}$	$ n_{Wapo}$	$n_{101,Wapo}$	$\hat{N}_{Wapo}^{\rm ML}$	\hat{N}_{Wapo}^{Chap}	$\Delta^{\rm Chap-ML}_{Wapo}$
1	1,956	134.07	4,279	4,263	-16	388	8.10	787	678	-109
2	1,283	45.78	4,687	4,464	-223	211	4.03	993	750	-243
3	1,130	37.41	4,458	4,304	-154	164	2.56	760	582	-178
4	516	17.62	1,006	978	-28	97	1.52	170	147	-23
5	496	9.56	2,241	2,065	-176	76	0.90	333	245	-88
6	491	41.02	1,316	1,278	-38	123	3.65	325	264	-61
7	436	36.36	1,072	1,055	-17	102	2.82	243	202	-41
8	350	12.83	1,388	1,302	-86	52	1.11	279	204	-75
9	319	11.04	1,224	1,133	-91	57	1.24	314	226	-88
10	241	7.72	555	533	-22	45	0.66	92	77	-15
11	237	6.07	1,222	989	-233	47	0.63	311	198	-113
12	224	4.84	952	890	-62	35	0.46	142	107	-35
13	201	11.23	685	586	-99	55	1.02	181	130	-51
14	106	2.71	329	274	-55	25	0.29	66	48	-18
15	95	7.82	287	275	-12	28	0.90	89	70	-19
16	91	1.44	561	435	-126	17	0.17	104	65	-39
17	46	1.15	252	194	-58	9	0.14	72	45	-27
18	35	1.90	150	120	-30	11	0.24	50	34	-16
Total	8,253	390.57	26,664	25,138	-1,526	1,542	30.44	5,311	4,072	-1,239

Table 6: Estimated number of homeless people in The Netherlands in 2021, separated by men and women and 18 subgroups based on age, living in- or outside one of the four big Dutch cities and country of origin.

play a role. The fact that such a regularity condition for MSE is unknown is unfortunate, because some of the subgroups are quite small and so the risk of not meeting a potential regularity condition is not unrealistic. The data on homeless people in The Netherlands that were used for this section is not publicly available due to legal restrictions.

5 Discussion

In this paper we have derived the Chapman MSE-estimator and we have shown that, in terms of mean-bias correction, it outperforms a set of other bias-reduced MSE estimators known in literature. We showed both mathematically and in a simulation study that mean-bias correction in DSE is best achieved by means of the DSE estimator proposed by Chapman (1951) and later by Rivest and Lévesque (2001). Furthermore we showed how the Chapman-estimator can be derived in a different way than Chapman did. This derivation was extended towards multiple sources, which led to the Chapman MSE-estimator for saturated models. We developed the Chapman MSE-estimator such that it can be applied under both a saturated and restricted model. This generalisation was achieved by using the MPI and for a small set of different restricted models it was proven mathematically that this approach leads to bias-corrected estimators. We used a simulation study to investigate bias in a larger set of restricted models and we found that also for these models the Chapman MSE-estimator shows little or no bias.

The mathematical derivations and simulation studies in this paper show that for any

restricted model with three sources or a saturated model with any number of sources, the Chapman MSE-estimator is a bias-corrected estimator. We suspect that this result can be generalised towards any restricted model with any number of sources, although we did not provide a mathematical proof. We think that further research that proofs, or disproofs, our suspicion would be valuable.

The simulation studies also show that the Chapman MSE-estimator outperforms other estimators in terms of a smaller size of bias and SD, and thus RMSE, in particular when the estimated log-linear model has more interaction parameters. This advantage is important because in practice the model that is used is usually the result of some model selection procedure, which does not guarantee the selection of the correct model. When such a selection procedure selects a model with irrelevant parameters, this increases the variance of the population size estimate. This increase is less for the Chapman MSE-estimator than for the other estimators considered.

In Section 4 we applied the Chapman MSE-estimator to estimate the number of homeless people in The Netherlands for a series of years and compared these estimates with the ML estimates. For each year both estimates are based on the same log-linear model as discussed in Coumans et al. (2017). This comparison showed that the impact of biascorrection can be substantial, e.g., in our example the use of the Chapman MSE-estimator led to a Chapman MSE estimate that was between 9.3% and 25.4% lower for the total number of homeless people in The Netherlands, as compared to the corresponding MLestimator. This relative difference became even larger, going up to 51%, when we zoomed in on the subgroup of women.

The simulation studies and the example in Section 4 show that the difference between the Chapman MSE- and the standard ML-estimator can be substantial. This raises the question whether finite-sample bias correction should not have a more prominent role in the discussion on the robustness of MSE methodology and the accuracy of MSE estimates, which continues up till today (see e.g. Binette & Steorts, 2022; Silverman, 2020).

Finally, a topic that received little or no attention in MSE literature, but what would be valuable to investigate, is regularity conditions. Chapman gave a regularity condition for his DSE estimator, but similar regularity conditions for MSE estimators are unknown. This topic is also beyond the scope of this paper but we think that this is an important remaining problem for MSE estimators in general, including the Chapman MSE-estimator.

Software

All simulation studies in this paper are performed in the statistical software program R (R Core Team, 2022). All estimates are obtained with the glm() function, with family = poisson(link = "log"). Differences between the LP, ML, Chapman, Bailey, EB, RL and Chapman MSE estimates are the sole result of different input vectors \mathbf{n}^{est} . For the IND model the estimation results for the RL-estimator were verified with the function closedp.bc() with m = "Mt" from the R-package Rcapture (Rivest, 2022). The Cordeiro-, Firth- and Kosmidis-estimator (\hat{N}^{CFK}) were also calculated with the glm()

function, but with the additional settings method = "brglmFit" and type = "correction", type = "AS_mean" and type = "MPL_Jeffreys", respectively, which are part of the R-package brglm2 (Kosmidis & Kenne Pagui, 2023). Code for the simulation studies presented in this paper is available at https://github.com/DaanZult/ChapmanMSE/.

Author contributions statement

D.Z. derived the Chapman MSE-estimator, did the set up and programming of the simulation studies, and wrote the manuscript. P.H. had the initial idea for the study and edited the manuscript. B.B. edited the manuscript.

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A Comparison of Taylor approximation and Stephan's inverse factorial approximation

The Taylor expansion that was also used by Bailey (1951) is a widely used approximation approach, but it is not always the most accurate or efficient method to approximate a function. To illustrate that the inverse factorial (IF) expansion (see e.g. Stephan, 1945) used by Chapman (1951) gives more accurate results for $\mathbb{E}\left[\frac{1}{n_{11}}\right]$, given the same number of expansion terms, than a Taylor expansion, we provide a straightforward simulation study. With r replications of $n_{11,r} \sim \text{Poisson}(m_{11})$, we can write five-term expansion Taylor and IF approximations for $\mathbb{E}\left[\frac{1}{n_{11}}\right]$ as

Taylor
$$\to \mathbb{E}\left[\frac{1}{n_{11}}\right] = \mathbb{E}\left[\frac{1}{m_{11}} - \frac{(n_{11} - m_{11})}{m^2} + \frac{(n_{11} - m_{11})^2}{m_{11}^3} - \frac{(m_{11} - n_{11})^3}{m_{11}^4} + \frac{(m_{11} - n_{11})^4}{m_{11}^5} - \dots\right]$$

where m_{11} will be estimated by $\hat{m}_{11} = \sum_r n_{11,r}/r$, and

$$\begin{split} \mathrm{IF} \to \mathbb{E} \left[\frac{1}{n_{11}} \right] &\approx \sum_{r} \left(\frac{1}{n_{11,r} + 1} \right) / r + \sum_{r} \left(\frac{1}{(n_{11,r} + 1) (n_{11,r} + 2)} \right) / r + \\ &\sum_{r} \left(\frac{2}{(n_{11,r} + 1) (n_{11,r} + 2) (n_{11,r} + 3)} \right) / r + \\ &\sum_{r} \left(\frac{6}{(n_{11,r} + 1) (n_{11,r} + 2) (n_{11,r} + 3) (n_{11,r} + 4)} \right) / r + \\ &\sum_{r} \left(\frac{24}{(n_{11,r} + 1) (n_{11,r} + 2) (n_{11,r} + 3) (n_{11,r} + 4) (n_{11,r} + 5)} \right) / r \end{split}$$

Table A1 shows the results for both approximation methods and their difference Δ for $m_{11} = 20$ and r = one million.

Table A1: Simulated approximations of $\mathbf{E}\left[\frac{1}{n_{11}}\right]$, with $n_{11,r} \sim \text{Poisson}(m_{11} = 20)$ and r = one million, which gives $\mathbf{E}\left[\frac{1}{n_{11}}\right] \approx \left(\sum_{r} \frac{1}{n_{11,r}}\right)/r = 0.052805$.

# Terms	Taylor	$\Delta(\mathbf{E}\left[\frac{1}{n_{11}}\right] - \mathbf{Taylor})$	IF	$\Delta(\mathbf{E}\left[\frac{1}{n_{11}}\right] - \mathbf{IF})$
1	0.050001	0.002804	0.050006	0.002799
2	0.050001	0.002804	0.052507	0.000298
3	0.052505	0.000299	0.052757	0.000048
4	0.052379	0.000426	0.052794	0.000010
5	0.052763	0.000042	0.052802	0.000003

Table A1 shows that, for $n_{11,r} \sim \text{Poisson}(m_r = 20)$ and five or less expansion terms, the IF approximation method used by Chapman (1951) gives a more accurate approximation

of $\mathbf{E}\left[\frac{1}{n_{11}}\right] \approx \left(\sum_{r} \frac{1}{n_{11,r}}\right)/r = 0.052805$ than the Taylor approximation method.

B Second-order Taylor approximation of the Lincoln-Petersen-estimator

Here we present an alternative derivation of a bias-reduced LP-estimator. This derivation shows that the Chapman-estimator can be approximated with the well-known Taylor approximation. We write the LP-estimator as a Taylor series approximation. When we start with some function $f(\mathbf{n})$ of the three random variables n_{11} , n_{10} and n_{01} , and approximate it around \mathbf{m} , this gives:

$$f(\mathbf{n}) = f(\mathbf{m}) + (\mathbf{n} - \mathbf{m})^{\top} \nabla f(\mathbf{m}) + \frac{1}{2} (\mathbf{n} - \mathbf{m})^{\top} \nabla \nabla f(\mathbf{m}) (\mathbf{n} - \mathbf{m}) + O(||(\mathbf{n} - \mathbf{m})^{\top}||)^2)$$

with

$$\nabla f(\mathbf{m}) = \begin{pmatrix} \frac{\partial f(\mathbf{n})}{\partial n_{11}} \\ \frac{\partial f(\mathbf{n})}{\partial n_{10}} \\ \frac{\partial f(\mathbf{n})}{\partial n_{01}} \end{pmatrix}_{\mathbf{m}}$$

and

$$\nabla \nabla f(\mathbf{m}) = \begin{pmatrix} \frac{\partial^2 f(\mathbf{n})}{\partial n_{11}^2} & \frac{\partial^2 f(\mathbf{n})}{\partial n_{11} \partial n_{10}} & \frac{\partial^2 f(\mathbf{n})}{\partial n_{11} \partial n_{01}} \\ \frac{\partial^2 f(\mathbf{n})}{\partial n_{10} \partial n_{11}} & \frac{\partial^2 f(\mathbf{n})}{\partial n_{10}^2} & \frac{\partial^2 f(\mathbf{n})}{\partial n_{10} \partial n_{01}} \\ \frac{\partial^2 f(\mathbf{n})}{\partial n_{01} \partial n_{11}} & \frac{\partial^2 f(\mathbf{n})}{\partial n_{01} \partial n_{10}} & \frac{\partial^2 f(\mathbf{n})}{\partial n_{01}^2} \end{pmatrix}_{\mathbf{m}}$$

Replacing $f(\mathbf{n})$ with $\hat{m}_{00}^{\text{LP}} = \frac{n_{10}n_{01}}{n_{11}}$ gives:

$$\nabla f(\mathbf{n}) = \begin{pmatrix} -\frac{n_{10}n_{01}}{n_{11}^2} \\ \frac{n_{10}}{n_{11}} \\ \frac{n_{01}}{n_{11}} \end{pmatrix}$$

and

$$\nabla \nabla f(\mathbf{n}) = \begin{pmatrix} \frac{2n_{10}n_{01}}{n_{11}^3} & -\frac{n_{01}}{n_{11}^2} & -\frac{n_{10}}{n_{11}^2} \\ -\frac{n_{01}}{n_{11}^2} & 0 & \frac{1}{n_{11}} \\ -\frac{n_{10}}{n_{11}^2} & \frac{1}{n_{11}} & 0 \end{pmatrix}.$$

Therefore, because $\mathbb{E}\left[(\mathbf{n} - \mathbf{m})^\top \nabla f(\mathbf{m})\right] = 0$, we find:

$$\mathbb{E}\left[\frac{n_{10}n_{01}}{n_{11}}\right] \approx \frac{m_{10}m_{01}}{m_{11}} + \frac{\operatorname{Cov}\left(n_{10}, n_{01}\right)}{m_{11}} - \frac{m_{10}\operatorname{Cov}\left(n_{11}, n_{01}\right)}{m_{11}^{2}} - \frac{m_{01}\operatorname{Cov}\left(n_{11}, n_{10}\right)}{m_{11}^{2}} + \frac{m_{10}m_{01}\operatorname{Var}\left(n_{11}\right)}{m_{11}^{3}}.$$
(33)

For the Poisson distribution we have $\text{Cov}(n_{ab}, n_{\neq ab}) = 0$ and $\text{Var}(n_{ab}) = m_{ab}$, and for the multinomial distribution we have $\text{Cov}(n_{ab}, n_{\neq ab}) = -Np_{ab}p_{\neq ab}$ and $\text{Var}(n_{ab}) = Np_{ab}(1 - p_{ab})$ with $p_{ab} = m_{ab}/N$. Then, for both $n_{ab} \sim \text{Poisson}(m_{ab})$ and the joint set $(n_{11}, n_{10}, n_{01}, n_{00}) \sim$ Multinomial $(m_{11}, m_{10}, m_{01}, m_{00})$, Eq. (33) reduces to:

$$\mathbb{E}\left[\frac{n_{10}n_{01}}{n_{11}}\right] \approx \frac{m_{11}m_{10}m_{01} + m_{10}m_{01}}{m_{11}^2} = \frac{m_{10}m_{01}}{m_{11}}\frac{m_{11} + 1}{m_{11}}.$$
(34)

This implies that $\mathbb{E}\left[\frac{n_{10}n_{01}}{n_{11}}\right]\frac{m_{11}}{m_{11}+1}$ removes the second-order Taylor approximation bias from the LP-estimator, which suggests that multiplying the LP-estimator with $\frac{n_{11}}{n_{11}+1}$, which gives the Chapman-estimator, is an improvement over the LP-estimator.

C Tables with SDs and RMSEs

C.1 DSE

S	SD ^{LP}	SD ^{Bailey}	SD ^{EB/CFK}	SD ^{Chap/RL}	RMSE ^{LP}	RMSE ^{Bailey}	RMSE ^{EB/CFK}	RMSE ^{Chap/RL}
1	27.8^{\dagger}	20.8	25.8	21.9	28.3 [†]	21.2	26.3	21.9
2	28.7	22.2	26.3	23.0	29.3	22.3	26.8	23.0
3	70.2	65.6	68.9	66.5	70.7	65.9	69.3	66.5
4	85.7	78.9	83.3	79.7	86.5	79.0	83.8	79.7
5	460.9	457.9	459.9	458.4	461.2	458.1	460.1	458.4
6	411.3	409.3	410.7	409.6	411.7	409.3	410.9	409.6
7	109.6†	45.8	104.2	48.8	118.9 [†]	47.5	107.9	49.4

Table C1: The SDs and RMSEs for the simulation study presented in Table 1.

A † as superscript indicates that extremely high estimates due to failures were replaced with the highest Chapman estimate in the simulation sample.

C.2 MSE with saturated models

S	$\mid N$	SD ^{ML,SAT}	SD ^{EB,SAT}	SD ^{CFK,SAT}	SD ^{RL,SAT}	SD ^{Chap MSE,SAT}
1	100	47.0^{\dagger}	54.7	40.2	29.6	23.6
2	500	103.9	102.4	101.0	93.9	89.4
3	10,000	364.2	364.1	364.0	362.8	362.1
4	100	58.5 [†]	72.5	46.9	33.3	25.4
5	500	111.9	109.6	107.5	99.9	94.6
6	10,000	373.4	373.2	373.0	371.9	371.2
7	100	76.9 [†]	86.4	51.1	34.1	24.7
8	500	139.9	132.6	126.8	114.7	105.6
9	10,000	391.8	391.6	391.4	390.0	389.1
10	100	66.5 [†]	71.4	44.7	30.5	22.7
11	500	128.8^{\dagger}	134.3	123.4	111.2	103.0
12	10,000	394.5	394.3	394.1	392.7	391.8
13	20,000	636.7	636.5	635.9	635.4	628.6
14	20,000	725.3	725.0	724.4	723.5	714.3

Table C2: The SDs of the estimates for saturated MSE models, as presented in Table 3.

A † as superscript indicates that extremely high estimates due to failures were replaced with the highest Chapman MSE estimate in the simulation sample.

S	$\mid N$	RMSEs ^{ML,SAT}	RMSEs ^{EB,SAT}	RMSEs ^{CFK,SAT}	RMSEs ^{RL,SAT}	RMSEs ^{Chap MSE,SAT}
1	100	48.7^{\dagger}	56.1	41.7	29.8	23.6
2	500	106.0	104.6	103.2	94.1	89.4
3	10,000	364.5	364.4	364.3	362.8	362.1
4	100	60.5^{\dagger}	73.9	48.4	33.4	25.4
5	500	114.7	112.3	110.1	100.2	94.6
6	10,000	373.7	373.5	373.4	371.9	371.2
7	100	79.8 [†]	88.4	52.8	34.3	24.7
8	500	143.5	136.1	130.2	115.1	105.6
9	10,000	392.3	392.1	392.0	390.1	389.1
10	100	68.8^{\dagger}	73.1	46.2	30.6	22.8
11	500	132.2 [†]	137.6	126.9	111.6	103.0
12	10,000	394.9	394.8	394.7	392.7	391.7
13	20,000	638.8	638.6	638.0	636.8	628.6
14	20,000	726.9	726.8	726.2	724.6	714.3

Table C3: The RMSEs of the estimates for saturated MSE models, as presented in Table 3.

A † as superscript indicates that extremely high estimates due to failures were replaced with the highest Chapman MSE estimate in the simulation sample.

C.3 MSE with restricted models

Table C4: The SDs of the estimates for the correct restricted MSE models, as presented in Table 5.

S	N	$\mathrm{SD}^{\mathrm{ML},\mathrm{LLM}^+}$	SD ^{EB,LLM+}	SD ^{CFK,LLM+}	$\mathrm{SD}^{\mathrm{RL},\mathrm{LLM}^+}$	SD ^{Chap MSE,LLM+}
1	100	8.0	7.9	8.0	8.0	7.8
2	500	28.5	28.3	28.5	28.4	28.3
3	10,000	125.9	125.8	125.8	125.8	125.8
4	100	11.7	11.4	11.6	10.9	11.0
5	500	41.2	40.7	41.0	40.1	40.3
6	10,000	164.4	164.3	164.3	164.2	164.2
7	100	15.4^{\dagger}	15.4	14.3	13.1	12.3
8	500	48.3	47.9	47.5	46.6	45.8
9	10,000	192.8	192.8	192.7	192.5	192.4
13	20,000	116.3	116.3	116.3	116.3	116.3
14	20,000	175.3	175.3	175.3	175.2	175.2

A † as superscript indicates that extremely high estimates due to failures were replaced with the highest Chapman estimate in the simulation sample.

S	$\mid N$	RMSE ^{ML,LLM+}	RMSE ^{EB,LLM+}	RMSE ^{CFK,LLM+}	RMSE ^{RL,LLM+}	RMSE ^{Chap MSE,LLM+}
1	100	8.0	8.0	8.1	8.0	7.8
2	500	28.6	28.3	28.6	28.4	28.3
3	10,000	125.9	125.8	125.9	125.8	125.8
4	100	11.8	11.4	11.8	10.9	11.0
5	500	41.4	40.8	41.2	40.1	40.3
6	10,000	164.4	164.3	164.4	164.2	164.2
7	100	15.7 [†]	15.7	14.6	13.2	12.3
8	500	48.6	48.2	47.8	46.6	45.8
9	10,000	192.9	192.8	192.8	192.6	192.4
13	20,000	116.3	116.3	116.3	116.3	116.3
14	20,000	175.3	175.3	175.3	175.2	175.2

Table C5: The RMSEs of the estimates for the correct restricted MSE models, as presented in Table 5.

A † as superscript indicates that extremely high estimates due to failures were replaced with the highest Chapman estimate in the simulation sample.