Improving the Accuracy of Estimating Indexes in Contingency Tables Using Bayesian Estimators

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Abstract
In contingency table analysis, one is interested in testing whether a model of interest (e.g., the independent or symmetry model) holds using goodness-of-fit tests. When the null hypothesis where the model is true is rejected, the interest turns to the degree to which the probability structure of the contingency table deviates from the model. Many indexes have been studied to measure the degree of the departure, such as the Yule coefficient and Cramér coefficient for the independence model, and Tomizawa’s symmetry index for the symmetry model. The inference of these indexes is performed using sample proportions, which are estimates of cell probabilities, but it is well known that the bias and mean square error (MSE) values become large without a sufficient number of samples. To address the problem, this study proposes a new estimator for indexes using Bayesian estimators of cell probabilities. Assuming the Dirichlet distribution for the prior of cell probabilities, we asymptotically evaluate the value of MSE, when plugging the posterior means of cell probabilities into the index, and propose an estimator of the index using the Dirichlet hyperparameter that minimizes the value. Numerical experiments show that when the number of samples per cell is small, the proposed method has smaller values of bias and MSE than other methods of correcting estimation accuracy. We also show that the values of bias and MSE are smaller than those obtained by using the uniform and Jeffreys priors.

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1 Introduction

For two-way contingency tables, an analysis is generally performed to determine whether the independence between the row and column classifications holds. Meanwhile, for the analysis of square contingency tables with the same row and column classifications, there are many issues related to symmetry rather than independence. This is because, in square contingency tables, there is a strong association between the row and column classifications. Bowker [5] proposed the symmetry model. Many other models for symmetry and asymmetry have been proposed, such as marginal homogeneity [18], quasi-symmetry [6], conditional symmetry [14], and diagonals-parameter symmetry [11]. For details, see Tahata and Tomizawa [19].

In the analysis of two-way contingency tables, the degree of departure from independence is measured using indexes between the row and column variables. These indexes include Yule’s coefficients of association and colligation [30, 31], Cramér’s coefficient [7], and Goodman and Kruskal’s coefficient [12]. For details, see Bishop et al [4] and Agresti [1]. Tomizawa et al [23] generalized Goodman and Kruskal’s coefficient via the power-divergence [8]. Tomizawa et al [26] also generalized Cramér’s coefficient via diversity index.

In addition, in the analysis of square contingency tables with the same row and column classifications, we are interested in measuring the degree of departure from symmetry or asymmetry. Over the past few years, many studies have proposed indexes to represent the degree of departure from symmetry or asymmetry. For square contingency tables with nominal categories, Tomizawa et al [24] and Tomizawa and Makii [22] proposed indexes based on the power-divergence and diversity index [15] to represent the degree of departure from the symmetry and marginal homogeneity models, respectively. For square contingency tables with ordered categories, Tomizawa et al [25] and Tomizawa et al [27] proposed indexes based on the power-divergence and diversity index to represent the degree of departure from the symmetry and diagonals-parameter symmetry models, respectively.

Although these indexes are estimated using sample proportions, which are typical estimators of cell probabilities, it is well known that the bias and mean squared error (MSE) values become large when the number of samples is not sufficient relative to the number of cells. To solve this problem, Tomizawa et al [28], Tahata et al [20], and Tahata et al [21] derived higher orders of bias and performed bias corrections. They showed numerical experiments that the improved estimators approached the true values of the indexes faster than the estimators with sample proportions as the sample size increases. However, although the improved estimators certainly reduce the value of bias, they do not necessarily reduce the value of MSE, that is, the variances of the estimators may become large. In addition, due to the bias correction term, the range of possible values for these improved estimators is not equal to that of their
corresponding indexes. For example, the value of Tomizawa et al [24]’s symmetry index lies between 0 and 1, but the value range of the improved estimator is beyond the range of 0 to 1. If the value of the improved estimator is outside the value range of the index, it would be difficult for analysts to interpret the value. It is also difficult to derive the asymptotic distribution of the improved estimator. Therefore, it is noted that the uncertainty quantification of the index based on the improved estimator may not be possible.

To solve further problems of the improved estimator in the estimation of indexes, we propose a newly inference method of indexes that improves the problems of their improved estimator, based on their idea of bias correction by deriving higher order of bias in the index itself rather than in the cell probabilities. Namely, we asymptotically evaluate the MSE of the estimator of index using the posterior means of the cell probabilities with the Dirichlet prior instead of sample proportions and derive the Dirichlet hyperparameter that minimizes the MSE. Our proposed estimator of indexes is constructed based on the posterior means of the cell probabilities with the derived Dirichlet parameter. The uncertainty quantification of the indexes in our proposed method can be easily performed by using the Monte Carlo simulation.

In a sense, this study may solve the problem of which the Dirichlet parameter can be used for precise estimation of indexes. There are many studies on the choice of Dirichlet parameters for estimating cell probabilities. One of the most famous is the uniform prior Dirichlet(1, . . . , 1), which originated in Bayes [2], and the Jeffreys prior Dirichlet(1/2, . . . , 1/2), derived from the invariance rule by Jeffreys [13]. With k the number of cells, Dirichlet(1/k, . . . , 1/k) was originally suggested by Perks [16] and recommended as an “overall objective” prior by Berger et al [3]. Fienberg and Holland [9] evaluated the variation of the risks of the posterior means of the cell probabilities with respect to the Dirichlet parameters. Fienberg and Holland [10] derived the Dirichlet parameters that asymptotically minimize the MSEs of the posterior means of the cell probabilities. Other studies, such as Tuyl [29], have discussed the choice of Dirichlet parameters in various situations, such as when there are many zero cells. Thus, there are many studies on the method of selecting the Dirichlet parameters in estimating cell probabilities other than those mentioned above, but to our knowledge, there is no study that discusses how to select the Dirichlet parameters to improve the accuracy of the estimation of indexes in contingency tables. Our contribution is not only to improve the accuracy of the estimation of index in contingency tables, but also to provide a method for selecting the Dirichlet hyperparameter when using Bayesian estimators of cell probabilities for the estimation of index.

This paper is organized as follows: Section 2 asymptotically evaluates the MSE of the estimator of the index with the posterior means of the cell probabilities and derives the Dirichlet parameter that asymptotically minimizes the MSE. Section 3 shows that the proposed estimators can reduce the bias and MSE more than other estimators in the numerical experiments. Section 4 presents the concluding remarks.
2 Dirichlet Parameter that Asymptotically Minimizes the MSE

Consider an \( r \times c \) contingency table. Suppose that \( n = (n_{11}, n_{12}, \ldots, n_{1c}, n_{21}, \ldots, n_{rc})^\top \) is a random vector with a multinomial distribution:

\[
p(n \mid p) = \frac{n!}{\prod_{i,j} n_{ij}!} \prod_{i,j} p_{ij}^{n_{ij}},
\]

where \( n = \sum_{i,j} n_{ij} \), \( p_{ij} \) is the probability that an observation falls in the \( i \)th row and \( j \)th column of the table (\( i = 1, \ldots, r \); \( j = 1, \ldots, c \)), \( p = (p_{11}, p_{12}, \ldots, p_{1c}, p_{21}, \ldots, p_{rc})^\top \), and \( b^\top \) is the transpose of \( b \). Let \( p \) have a Dirichlet prior density

\[
p(p \mid \alpha) = \frac{\Gamma(r c \alpha)}{(\Gamma(\alpha))^r c} \prod_{i,j} p_{ij}^{\alpha-1},
\]

where \( \Gamma(\cdot) \) is the Gamma function. In this case, the posterior distribution of \( p \) is

\[
p(p \mid n) = \frac{\Gamma(\sum_{i,j} (\alpha + n_{ij}))}{\prod_{i,j} \Gamma(\alpha + n_{ij})} \prod_{i,j} p_{ij}^{n_{ij}+\alpha-1},
\]

so the posterior mean of \( p \) is

\[
\hat{p}^{(\alpha)} = (\hat{p}_{11}^{(\alpha)}, \hat{p}_{12}^{(\alpha)}, \ldots, \hat{p}_{1c}^{(\alpha)}, \hat{p}_{21}^{(\alpha)}, \ldots, \hat{p}_{rc}^{(\alpha)})^\top,
\]

where

\[
\hat{p}_{ij}^{(\alpha)} = \frac{n_{ij} + \alpha}{n + r c \alpha}.
\]

When \( \alpha = 0 \), the posterior mean \( \hat{p}_{ij}^{(\alpha)} \) corresponds to the sample proportion \( \hat{p}_{ij} = n_{ij}/n \). When we adopt the squared distance from the estimator to \( p \) as the loss function, \( \hat{p}^{(\alpha)} \) is the Bayes estimator of \( p \).

Let a function \( f(\cdot) \) denote an index in contingency tables. Many indexes in contingency tables that have been proposed thus far are defined as functions of \( p \). Therefore, the value of the index \( f(p) \) is estimated using \( f(\hat{p}) \), where \( p \) is replaced by the sample proportions \( \hat{p} \) in \( f(p) \). In this study, instead of \( f(\hat{p}) \), \( f(\hat{p}^{(\alpha)}) \), where \( p \) is replaced by \( \hat{p}^{(\alpha)} \) in \( f(p) \) is considered as an estimator of an index, and in order to improve the accuracy for estimating the index, we asymptotically evaluate the MSE of \( f(\hat{p}^{(\alpha)}) \) and derive the Dirichlet parameter that minimizes it.

First, we consider the Dirichlet parameter as follows:

\[
\alpha^* = \arg\min_{\alpha} \lim_{n \to \infty} n^2 \text{MSE}[f(\hat{p}^{(\alpha)})].
\]

Here, the following theorems hold.
Theorem 1 Suppose that $f(\cdot)$ is at least four times differentiable at $p$. The MSE of $f(\hat{p}^{(\alpha)})$ is expressed as

$$\text{MSE}[f(\hat{p}^{(\alpha)})] = \frac{1}{n^2} \left( A_1 \alpha^2 - 2 A_2 \alpha \right) + \text{(terms independent of } \alpha) + o(n^{-2}),$$

where

$$A_1 = \text{tr} \left[ \left( \frac{\partial f(p)}{\partial p} \right) \left( \frac{\partial f(p)}{\partial p^\top} \right) (rcp - 1_{rc})(rcp - 1_{rc})^\top \right],$$

$$A_2 = \frac{1}{2} (rcp - 1_{rc})^\top \left( \frac{\partial f(p)}{\partial p} \right) \text{tr} \left[ \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) (\text{diag}(p) - pp^\top) \right]$$

$$+ rc \text{ tr} \left[ \left( \frac{\partial f(p)}{\partial p} \right) \left( \frac{\partial f(p)}{\partial p^\top} \right) (\text{diag}(p) - pp^\top) \right],$$

$$+ \text{ tr} \left[ \left( \frac{\partial f(p)}{\partial p} \right) (rcp - 1_{rc})^\top \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) (\text{diag}(p) - pp^\top) \right].$$

$1_{rc}$ is the $rc \times 1$ vector with all elements equal to one, and $\text{diag}(p)$ is a diagonal matrix with the elements of $p$ on the main diagonal.

Proof The MSE of $f(\hat{p}^{(\alpha)})$ is expressed as

$$\text{MSE}[f(\hat{p}^{(\alpha)})] = \mathbb{E}[(f(\hat{p}^{(\alpha)}) - f(p))^2]$$

$$= \mathbb{E}[(f(\hat{p}^{(\alpha)}) - f(\hat{p}))(f(\hat{p}^{(\alpha)}) - f(\hat{p}))^2].$$

Because $f(\cdot)$ is at least four times differentiable at $p$, $f(\hat{p})$ is expressed as

$$f(\hat{p}) = f(p) + \frac{1}{\sqrt{n}} \left( \frac{\partial f(p)}{\partial p^\top} \right) u + \frac{1}{2n} u^\top \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) u$$

$$+ \frac{1}{6n^{3/2}} \left( \sum_{i,j} \sum_{k,l} \sum_{s,t} u_{ij} u_{kl} u_{st} \frac{\partial^3}{\partial p_{ij} \partial p_{kl} \partial p_{st}} \right) f(p) + O_p(n^{-2}),$$

where $u = (u_{11}, u_{12}, \ldots, u_{1c}, u_{21}, \ldots, u_{rc})^\top$ and $u_{ij} = \sqrt{n}(\hat{p}_{ij} - p_{ij})$. It should be noted that $u \sim \mathcal{N}(\hat{p} - p)$ as $n \rightarrow \infty$.

Additionally, $f(\hat{p}^{(\alpha)})$ is expressed as

$$f(\hat{p}^{(\alpha)}) = f(\hat{p}) + \left( \frac{\partial f(\hat{p})}{\partial p^\top} \right) (\hat{p}^{(\alpha)} - \hat{p}) + O_p(n^{-2})$$

$$= f(\hat{p}) - \frac{\alpha}{n} \left( \frac{\partial f(p)}{\partial p^\top} \right) (rcp - 1_{rc}).$$

$$- \frac{\alpha}{n^{3/2}} u^\top \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) (rcp - 1_{rc}) - \frac{rc\alpha}{n^{3/2}} \left( \frac{\partial f(p)}{\partial p^\top} \right) u + O_p(n^{-2}).$$
since
\[
\frac{\partial f(\hat{p})}{\partial \hat{p}^\top} = \frac{\partial f(p)}{\partial p^\top} + \frac{1}{\sqrt{n}} u^\top \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) + O_p(n^{-1})
\]
and
\[
\hat{p}^{(\alpha)}_{ij} = \frac{n_{ij}}{n} \left( \frac{1}{1 + n^{-1} rc\alpha} \right) + \frac{\alpha}{n} \left( \frac{1}{1 + n^{-1} rc\alpha} \right)
\]
\[
= \hat{p}_{ij} \left( 1 - \frac{rc\alpha}{n} + O(n^{-2}) \right) + \frac{\alpha}{n} \left( 1 - \frac{rc\alpha}{n} + O(n^{-2}) \right)
\]
\[
= \hat{p}_{ij} - \frac{rc\alpha}{n} \hat{p}_{ij} + \frac{\alpha}{n} + O_p(n^{-2})
\]
\[
= \hat{p}_{ij} - \frac{rc\alpha}{n} (rcp_{ij} - 1) - \frac{rc\alpha}{n^{3/2}} \sqrt{n}(\hat{p}_{ij} - p_{ij}) + O_p(n^{-2}).
\]

From Eqs. (1), (2), and (3), we have
\[
f(\hat{p}^{(\alpha)}) - f(p) = \frac{1}{\sqrt{n}} F_1 + \frac{1}{n} (F_{21} - \alpha F_{22}) + \frac{1}{n^{3/2}} (F_{31} - \alpha F_{32} - \alpha F_{33}) + O_p(n^{-2}),
\]
where
\[
F_1 = \left( \frac{\partial f(p)}{\partial p^\top} \right) u, \quad F_{21} = \frac{1}{2} u^\top \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) u, \quad F_{22} = \left( \frac{\partial f(p)}{\partial p^\top} \right) (rcp - 1_{rc}),
\]
\[
F_{31} = \frac{1}{6} \left( \sum_{i,j} \sum_{k,l} \sum_{s,t} u_{ij} u_{kl} u_{st} \frac{\partial^3}{\partial p_{ij} \partial p_{kl} \partial p_{st}} f(p) \right), \quad F_{32} = rc \left( \frac{\partial f(p)}{\partial p^\top} \right) u,
\]
\[
F_{33} = u^\top \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) (rcp - 1_{rc})
\]
and then the MSE of \( f(\hat{p}^{(\alpha)}) \) is expressed as
\[
\text{MSE}[f(\hat{p}^{(\alpha)})] = \frac{1}{n} \mathbb{E}[F_1^2] + \frac{2}{n^{3/2}} \mathbb{E}[F_1 (F_{21} - \alpha F_{22})]
\]
\[
+ \frac{1}{n^2} \mathbb{E}[(F_{21} - \alpha F_{22})^2] + \frac{2}{n^{3/2}} \mathbb{E}[F_1 (F_{31} - \alpha F_{32} - \alpha F_{33})] + o(n^{-2})
\]
\[
= \frac{1}{n^2} \left( A_1 \alpha^2 - 2A_2 \alpha \right) + A_3 + o(n^{-2}),
\]
where

\[ A_1 = \text{tr} \left[ \left( \frac{\partial f(p)}{\partial p} \right) \left( \frac{\partial f(p)}{\partial p^\top} \right) (r_c p - 1_{r_c}) (r_c p - 1_{r_c})^\top \right], \]

\[ A_2 = \frac{1}{2} (r_c p - 1_{r_c})^\top \left( \frac{\partial f(p)}{\partial p} \right) \text{tr} \left[ \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) (\text{diag}(p) - pp^\top) \right] \]

\[ + r_c \text{tr} \left[ \left( \frac{\partial f(p)}{\partial p} \right) \left( \frac{\partial f(p)}{\partial p^\top} \right) (\text{diag}(p) - pp^\top) \right], \]

\[ + \text{tr} \left[ \left( \frac{\partial f(p)}{\partial p} \right) (r_c p - 1_{r_c})^\top \left( \frac{\partial^2 f(p)}{\partial p \partial p^\top} \right) (\text{diag}(p) - pp^\top) \right], \]

\[ A_3 = \frac{1}{n} \mathbb{E}[F_1^2] + \frac{2}{n^{3/2}} \mathbb{E}[F_1 F_{21}] + \frac{1}{n^2} \mathbb{E}[F_{21}^2] + \frac{2}{n^2} \mathbb{E}[F_1 F_{31}], \]

since

\[ \mathbb{E}[F_1 F_{22}] = (r_c p - 1_{r_c})^\top \left( \frac{\partial f(p)}{\partial p} \right) \left( \frac{\partial f(p)}{\partial p^\top} \right) \mathbb{E}[u] = 0. \]

Note that the terms in \( A_3 \) are independent of \( \alpha \). \( \square \)

**Theorem 2** The Dirichlet parameter \( \alpha \) that asymptotically minimizes the MSE of \( f(\hat{p}(\alpha)) \) is obtained as follows:

\[ \alpha^* = \text{argmin}_{\alpha} \lim_{n \to \infty} n^2 \text{MSE}[f(\hat{p}(\alpha))] = \frac{A_2}{A_1}. \]

From Theorem 1, it is clear that Theorem 2 holds.

Therefore, using

\[ \hat{\alpha}^* = \frac{\hat{A}_2}{\hat{A}_1}, \quad (4) \]

where \( \hat{A}_1 \) and \( \hat{A}_2 \) denote \( A_1 \) and \( A_2 \) with \( p \) replaced by \( \hat{p} \), respectively. We propose \( f(\hat{p}(\hat{\alpha}^*)) \) as an estimator of the index \( f(p) \).

### 3 Numerical Experiments

This section shows that the proposed estimator \( f(\hat{p}(\hat{\alpha}^*)) \) can reduce the bias and MSE more than the estimator with sample proportions \( f(\hat{p}) \) and the improved estimator (e.g., [28]) in the numerical experiments. We also show that the Dirichlet parameter \( \hat{\alpha}^* \) chosen by the proposed method (4) is more suitable for improving the accuracy for estimating indexes than other methods of choosing the Dirichlet parameter (e.g., \( \alpha = 1 \) (uniform prior), \( \alpha = 1/2 \) (Jeffreys prior), and Fienberg and Holland [10]’s method...
The bias and MSE based on the numerical experiments are calculated as

\[
\text{Bias} = \frac{1}{S} \sum_{i=1}^{S} f_i(p^*) - f(p), \quad \text{MSE} = \frac{1}{S} \sum_{i=1}^{S} (f_i(p^*) - f(p))^2,
\]

where \( S \) is the number of times a multinomial random number is generated, and \( f_i(p^*) \) is the estimated value of \( f(p) \) at the \( i \)th multinomial random number. These numerical experiments are performed using the programming language \( R \) [17].

### 3.1 Numerical Experiment for Index in Two-Way Contingency Tables

First, we consider the generalized Cramér’s coefficient in \( r \times c \) contingency tables. Tomizawa et al [26] proposed the generalized Cramér’s coefficient where the column variable is the explanatory variable and the row variable is the response variable as follows:

\[
f(p) = V^{(\lambda)} = \frac{I^{(\lambda)}(\{p_{ij}\}; \{p_i \cdot p \cdot j\})}{K^{(\lambda)}} \quad \text{for} \quad \lambda \geq 0,
\]

where

\[
I^{(\lambda)}(\{p_{ij}\}; \{p_i \cdot p \cdot j\}) = \frac{1}{\lambda(\lambda + 1)} \sum_{i,j} p_{ij} \left[ \left( \frac{p_{ij}}{p_i \cdot p \cdot j} \right)^\lambda - 1 \right],
\]

\[
p_i \cdot = \sum_j p_{ij}, \quad p \cdot j = \sum_i p_{ij}, \quad K^{(\lambda)} = \frac{1}{\lambda(\lambda + 1)} \left( \sum_i p_i^{1-\lambda} - 1 \right),
\]

and the value at \( \lambda = 0 \) is taken as the continuous limit as \( \lambda \to 0 \). Note that \( I^{(\lambda)}(\cdot; \cdot) \) is the power-divergence between two distributions \( \{p_{ij}\} \) and \( \{p_i \cdot p \cdot j\} \), including the Kullback–Leibler information (\( \lambda = 0 \)) and one-half of the Pearson chi-squared type discrepancy (\( \lambda = 1 \)), and the real number \( \lambda \) is chosen by the user. In this numerical experiment, we consider the case of \( \lambda = 1 \) for simplicity.

Suppose that \( 4 \times 5 \) contingency tables are generated 10,000 times by a multinomial random number based on the structures of probabilities in Table 1a–c. These probability tables are constructed so that the values are at both ends of the range of the generalized Cramér’s coefficient and in the middle of the range, in fact, these values for Table 1a–c are 0.091, 0.486, and 0.819, respectively.

Figures 1, 2, and 3 represent the absolute value of bias and MSE for several estimators of the generalized Cramér’s coefficient with Table 1 when \( \gamma = 1, 2, \ldots, 10 \), where \( \gamma \) is the proportion of sample size to the number of cells.

As can be seen from Figs. 1 and 2, the estimator with the sample proportions \( f(\hat{p}) \) (green line) has the large values of bias and MSE overall, while the values of bias and MSE are smaller in Fig. 3, because Table 1c has many cells with probabilities close to zero and the estimation accuracy of the sample proportions is good. Our proposed
estimator $f(\hat{p}(\hat{\alpha}^*))$ (red line) has significantly improved the estimation accuracy compared to the conventional estimator $f(\hat{p})$ (green line) in the situations of Table 1a and b, and has the same estimation accuracy as $f(\hat{p})$ in the situation of Table 1c, where $f(\hat{p})$ has the good estimation accuracy. It is also found that $f(\hat{p}(\hat{\alpha}^*))$ has the smaller values of the MSE than the improved estimator with bias correction (light blue line), although slightly. On the other hand, the improved estimator has the smaller values of the bias, but $f(\hat{p}(\hat{\alpha}^*))$ has the smaller bias value when $\gamma$ is small.

Comparing the estimators of the index using the Bayesian estimators of the cell probabilities with each other, in Fig. 1, the estimators with the posterior means of the cell probabilities using the uniform prior $f(\hat{p}(1))$ (pink line) and Jeffreys prior $f(\hat{p}(1/2))$ (brown line), and the estimator with the posterior means of the cell probabilities using the Dirichlet parameter chosen by Fienberg and Holland [10]'s method (yellow line) show almost the same estimation accuracy, and the values of bias and MSE are small, which may be due to the appropriate prior information. As the value of $\gamma$ increases, i.e., as the number of samples increases, the estimation accuracy of our proposed estimator $f(\hat{p}(\hat{\alpha}^*))$ becomes equal to or better than those estimators. Whereas, in Figs. 2, and 3, the values of the bias and MSE of $f(\hat{p}(1))$ (pink line), $f(\hat{p}(1/2))$ (brown line), and the estimator with the Dirichlet parameter chosen by Fienberg and Holland [10]'s method (yellow line) are much larger than those of $f(\hat{p})$. However, as mentioned above, our proposed estimator $f(\hat{p}(\hat{\alpha}^*))$ shows better estima-
Fig. 2 The absolute values of the bias and the values of MSE for several estimators of the generalized Cramér’s coefficient with Table 1 when \( \gamma = 1, 2, \ldots, 10 \), where \( \gamma \) is the proportion of sample size to the number of cells (Samp.Prop. (green line): plug-in estimator with the sample proportions; New (red line): the proposed estimator; Improved (light blue line): Improved estimator; FHM (yellow line): plug-in estimator with the posterior means of the cell probabilities using the Dirichlet parameter chosen by Fienberg and Holland [10]’s method; Uniform (pink line): plug-in estimator with the posterior means of the cell probabilities using the uniform prior; Jeffreys (brown line): plug-in estimator with the posterior means of the cell probabilities using Jeffreys prior).

Table 1 The 4 × 5 structures of probabilities to generate a multinomial random number

|       | (a)       | (b)       | (c)       |
|-------|-----------|-----------|-----------|
| 0.048 | 0.055     | 0.105     | 0.023     | 0.018 | 0.154 | 0.013 | 0.021 | 0.018 | 0.145 | 0.006 | 0.003 | 0.006 | 0.182 |
| 0.032 | 0.061     | 0.035     | 0.018     | 0.098 | 0.017 | 0.17 | 0.159 | 0.015 | 0.012 | 0.004 | 0.003 | 0.188 | 0.005 | 0.004 |
| 0.055 | 0.131     | 0.016     | 0.082     | 0.054 | 0.015 | 0.157 | 0.011 | 0.017 | 0.018 | 0.005 | 0.187 | 0.004 | 0.007 | 0.003 |
| 0.029 | 0.012     | 0.032     | 0.033     | 0.063 | 0.013 | 0.011 | 0.013 | 0.163 | 0.011 | 0.006 | 0.004 | 0.005 | 0.190 | 0.003 |

Estimation accuracy than \( f(\hat{p}) \) in Fig. 2 and the same accuracy as \( f(\hat{p}) \) in Fig. 3, indicating that it is the stable estimation method in all situations in Table 1.

3.2 Numerical Experiment for Index in Square Contingency Tables

Next, we consider a index to represent the degree of departure from the symmetry model in square contingency tables. Tomizawa et al [24] proposed the index to represent the degree of departure from the symmetry model as follows:

\[
f(p) = \Phi^{(\lambda)} = \sum_{i < j} (p_{ij}^* + p_{ji}^*) \Phi_{ij}^{(\lambda)} \text{ for } \lambda > -1,
\]
Fig. 3 The absolute values of the bias and the values of MSE for several estimators of the generalized Cramér’s coefficient with Table 1c when $γ = 1, 2, \ldots, 10$, where $γ$ is the proportion of sample size to the number of cells (Samp.Prop. (green line): plug-in estimator with the sample proportions; New (red line): the proposed estimator; Improved (light blue line): Improved estimator; FHM (yellow line): plug-in estimator with the posterior means of the cell probabilities using the Dirichlet parameter chosen by Fienberg and Holland [10]’s method; Uniform (pink line): plug-in estimator with the posterior means of the cell probabilities using the uniform prior; Jeffreys (brown line): plug-in estimator with the posterior means of the cell probabilities using Jeffreys prior)

where

$$\phi_{ij}^{(λ)} = 1 - \frac{λ^2}{2^λ - 1} H_{ij}^{(λ)}, \quad H_{ij}^{(λ)} = \frac{1}{λ} \left[ 1 - (p_{ij}^c)^{λ+1} - (p_{ji}^c)^{λ+1} \right],$$

$$p_{ij}^c = \frac{p_{ij}}{p_{ij} + p_{ji}}, \quad p_{ij}^\delta = \frac{p_{ij}}{\delta}, \quad \delta = \sum_{i \neq j} p_{ij},$$

and the value at $λ = 0$ is taken as the continuous limit as $λ \to 0$. Note that $H_{ij}^{(λ)}$ is the Patil and Taillie [15]’s diversity index of degree $λ$, including the Shannon entropy ($λ = 0$), and the real number $λ$ is chosen by the user. In this numerical experiment, we consider the case of $λ = 1$ for simplicity.

Suppose that $4 \times 4$ square contingency tables are generated 10,000 times by a multinomial random number based on the structures of probabilities in Tables 2a–c. These probability tables are constructed so that the values are at both ends of the range of the index for symmetry and in the middle of the range, in fact, these values for Table 2a–c are 0.099, 0.473, and 0.800, respectively. Additionally, we assume that contingency tables whose rows and columns consist of the same classification may have larger probabilities of the main diagonal cells.

Figures 4, 5, and 6 represent the absolute value of bias and MSE for several estimators of the index to represent the degree of departure from symmetry with Table
The absolute values of the bias and the values of MSE for several estimators of the index to represent the degree of departure from symmetry with Table 2a when $\gamma = 1, 2, \ldots, 10$, where $\gamma$ is the proportion of sample size to the number of cells (Samp.Prop. (green line): plug-in estimator with the sample proportions; New (red line): the proposed estimator; Improved (light blue line): Improved estimator; FHM (yellow line): plug-in estimator with the posterior means of the cell probabilities using the Dirichlet parameter chosen by Fienberg and Holland [10]’s method; Uniform (pink line): plug-in estimator with the posterior means of the cell probabilities using the uniform prior; Jeffreys (brown line): plug-in estimator with the posterior means of the cell probabilities using Jeffreys prior).

Similar to the numerical experiments in Sect. 3.1, the estimator with the sample proportions $f(\hat{p})$ (green line) has poor estimation accuracy in the case of Table 2a and b, which have few cells with zero probability (Figs. 4 and 5), but good accuracy in the case of Table 2c, which has many cells with zero probability (Fig. 6). In this numerical experimental setting, our proposed estimator $f(\hat{p}(\hat{\alpha}^*))$ (red line) also has significantly improved the estimation accuracy compared to the conventional estimator $f(\hat{p})$ (green line) in the situations of Table 2a and b, and has the same estimation accuracy as $f(\hat{p})$ in the situation of Table 2c, where $f(\hat{p})$ has the good estimation accuracy. It is also found that $f(\hat{p}(\hat{\alpha}^*))$ has the smaller values of the MSE than the improved estimator with bias correction (light blue line), although slightly. On the other hand, the improved estimator has the smaller values of the bias, but $f(\hat{p}(\hat{\alpha}^*))$ has the smaller bias value when $\gamma$ is small.

Comparing the estimators of the index using the Bayesian estimators of the cell probabilities with each other, in Fig. 4, the estimators with the posterior means of the cell probabilities using the uniform prior $f(\hat{p}^{(1)})$ (pink line) and Jeffreys prior $f(\hat{p}^{(1/2)})$ (brown line), and the estimator with the posterior means of the cell probabilities using the Dirichlet parameter chosen by Fienberg and Holland [10]’s method (yellow line) show almost the same estimation accuracy, and the values of bias and MSE are small, which may be due to the appropriate prior information. As the value...
The absolute values of the bias and the values of MSE for several estimators of the index to represent
the degree of departure from symmetry with Table 2 when \( \gamma = 1, 2, \ldots, 10 \), where \( \gamma \) is the proportion
of sample size to the number of cells (Samp.Prop. (green line): plug-in estimator with the sample proportions; New (red line): the proposed estimator; Improved (light blue line): Improved estimator; FHM (yellow line): plug-in estimator with the posterior means of the cell probabilities using the Dirichlet parameter chosen by Fienberg and Holland [10]’s method; Uniform (pink line): plug-in estimator with the posterior means of the cell probabilities using the uniform prior; Jeffreys (brown line): plug-in estimator with the posterior means of the cell probabilities using Jeffreys prior)

of \( \gamma \) increases, i.e., as the number of samples increases, the estimation accuracy of our proposed estimator \( f(\hat{\alpha}) \) becomes equal to or better than those estimators. Whereas, in Figs. 5, and 6, the values of the bias and MSE of \( f(\hat{p}(1)) \) (pink line) and the estimator with the Dirichlet parameter chosen by Fienberg and Holland [10]’s method (yellow line) are much larger than those of \( f(\hat{p}) \). In Fig. 5, the values of MSE of \( f(\hat{p}(1/2)) \) (brown line) are smaller, but the values of bias are larger, and in Fig. 6, the values of the bias and MSE of \( f(\hat{p}(1/2)) \) are much larger. However, as mentioned above, our proposed estimator \( f(\hat{p}(\hat{\alpha})) \) shows better estimation accuracy than \( f(\hat{p}) \) in Fig. 5 and the same accuracy as \( f(\hat{p}) \) in Fig. 6, indicating that it is the stable estimation method in all situations in Table 2.

Remark 1 As mentioned in Sect. 1, the range of value for the improved estimator does not equal the range of value for the index. This problem could be addressed by matching the range of value for the index with that of the improved estimator using a transformation based on the logit function or some other functions. Here, we describe the accuracy of the improved estimator with the logit transformation through the setting of numerical experiments in Sects. 3.1 and 3.2.

Tables 3 and 4 show the absolute values of the bias and the values of MSE for the improved estimators with the logit transformation of Tomizawa et al [26]’s and Tomizawa et al [24]’s indexes, \( V(\lambda) \) and \( \Phi(\lambda) \), when \( \gamma = 1, 2, \ldots, 10 \), where \( \gamma \) is the proportion of sample size to the number of cells, respectively. From these results, it is important to note that the values of the bias and MSE do not approach zero even when
The value of bias

The value of MSE

Method
- Samp.Prop.
- New
- Improved
- FHM
- Uniform
- Jeffreys

Fig. 6 The absolute values of the bias and the values of MSE for several estimators of the index to represent the degree of departure from symmetry with Table 2c when \( \gamma = 1, 2, \ldots, 10 \), where \( \gamma \) is the proportion of sample size to the number of cells (Samp.Prop. (green line): plug-in estimator with the sample proportions; New (red line): the proposed estimator; Improved (light blue line): Improved estimator; FHM (yellow line): plug-in estimator with the posterior means of the cell probabilities using the Dirichlet parameter chosen by Fienberg and Holland [10]’s method; Uniform (pink line): plug-in estimator with the posterior means of the cell probabilities using the uniform prior; Jeffreys (brown line): plug-in estimator with the posterior means of the cell probabilities using Jeffreys prior)

the value of \( \gamma \) increases, i.e., when the sample size increases given the fixed number of cells. While the improved estimator is the asymptotically unbiased estimator and thus the value of the bias approaches zero as the sample size increases, the improved estimator with the logit transformation is not the asymptotically unbiased estimator, as shown in these numerical experiments. The improved estimator, which is still the asymptotically unbiased estimator even after a certain transformation, is a subject for future work.

Remark 2 Here, we show how much the improved estimates does not fall within the interval \([0, 1]\) in the settings of the numerical experiments described above and in some additional probability structures.

Case 1: Tomizawa et al [26]’s index
Consider the probability tables in Table 5d and e in addition to those in Tables 1a–c. The values of the index \( V^{(\lambda)} \) in Table 5d and e are 0.006 and 0.971, respectively. The closer the value of the index is to the boundary of its range, the more likely the improved estimator is to be in the outside of the range. In fact, as shown in Table 6, the number of times that the improved estimate is in the outside of the range of the index for the five probability structures for 10,000 simulations is the highest for Table 5d at about 30%, followed by 10% for Table 5e. This occurs more frequently for smaller values of \( \gamma \), the proportion of the number of samples to the number of cells.

Case 2: Tomizawa et al [24]’s index
Table 2  The $4 \times 4$ structures of probabilities to generate a multinomial random number

|      | (a)  | (b)  | (c)  |
|------|------|------|------|
| 0.100| 0.060| 0.038| 0.071|
| 0.038| 0.100| 0.061| 0.026|
| 0.068| 0.051| 0.100| 0.031|
| 0.029| 0.066| 0.100| 0.071|

Table 3  The absolute values of the bias and the values of MSE for the improved estimator with the logit transformation of Tomizawa et al [26]'s index $V(\lambda)$ in Table 1a–e when $\gamma = 1, 2, \ldots, 10$, where $\gamma$ is the proportion of sample size to the number of cells

| $\gamma$ | Bias | MSE     |
|----------|------|---------|
| 1        | 0.454| 0.207   |
| 2        | 0.436| 0.190   |
| 3        | 0.434| 0.188   |
| 4        | 0.433| 0.187   |
| 5        | 0.432| 0.187   |
| 6        | 0.432| 0.187   |
| 7        | 0.432| 0.186   |
| 8        | 0.432| 0.186   |
| 9        | 0.432| 0.186   |
| 10       | 0.432| 0.186   |

Consider the probability tables in Table 7 in addition to those in Table 2a–c. The value of the index $\Phi(\lambda)$ in Table 7 is 0.993. As the result described in Case 1 for Tomizawa et al [26]'s index, Table 8 shows that the closer the value of the index is to the boundary of its range, the more frequently the improved estimates are in the outside of the range. In particular, in Table 2a, where the value of the index is close to 0, and in Table 7, where the value is close to 1, the improved estimates are in the outside of the range of the index for about 10% of the 10,000 simulations.

4 Concluding Remarks

This study solved the problem of poor estimation accuracy of the estimator of indexes with sample proportions without a sufficient number of samples, by using the Bayesian estimators of cell probabilities under the assumption of the Dirichlet prior. In doing so, we asymptotically evaluated the MSE of the estimator of indexes with the Bayesian estimators of cell probabilities and derived the Dirichlet parameter that minimizes the MSE.

Tomizawa et al. [28], Tahata et al. [20], and Tahata et al. [21] derived higher orders of bias and performed bias corrections, but the range of possible values for their estimators is not equal to that of their corresponding indexes, which made it difficult to interpret the values of the estimates and their confidence intervals. In addition,
Table 4 The absolute values of the bias and the values of MSE for the improved estimator with the logit transformation of Tomizawa et al [24]'s index $\Phi_1(\lambda)$ in Tables 2a–c, and 7 when $\gamma = 1, 2, \ldots, 10$, where $\gamma$ is the proportion of sample size to the number of cells

| $\gamma$ | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Bias     |     |     |     |     |     |     |     |     |     |     |
| Table 2a | 0.514 | 0.456 | 0.439 | 0.432 | 0.430 | 0.428 | 0.428 | 0.428 | 0.427 | 0.427 |
| Table 2b | 0.191 | 0.157 | 0.148 | 0.147 | 0.145 | 0.144 | 0.144 | 0.144 | 0.143 | 0.143 |
| Table 2c | 0.094 | 0.106 | 0.108 | 0.109 | 0.109 | 0.110 | 0.110 | 0.110 | 0.110 | 0.110 |
| MSE      |     |     |     |     |     |     |     |     |     |     |
| Table 2a | 0.268 | 0.211 | 0.194 | 0.188 | 0.186 | 0.184 | 0.184 | 0.183 | 0.183 | 0.183 |
| Table 2b | 0.040 | 0.027 | 0.024 | 0.023 | 0.022 | 0.021 | 0.021 | 0.021 | 0.021 | 0.021 |
| Table 2c | 0.010 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.012 | 0.012 |

Table 5 The 4 × 5 structures of probabilities to generate a multinomial random number

| (d) | (e) |
|-----|-----|
| 0.048 | 0.055 | 0.065 | 0.033 | 0.048 | 0.199 | .0005 | .0005 | .0005 | 0.198 |
| 0.032 | 0.061 | 0.048 | 0.038 | 0.068 | .0005 | 0.001 | 0.197 | 0.001 | .0005 |
| 0.045 | 0.071 | 0.046 | 0.042 | 0.054 | 0.001 | 0.198 | .0005 | .0005 | 0.001 |
| 0.049 | 0.052 | 0.049 | 0.033 | 0.063 | .0005 | .0005 | 0.001 | 0.198 | .0005 |

Table 6 The number of times that the improved estimate is in the outside of the range of Tomizawa et al [26]'s index $V^{(\lambda)}$ for Table 1a–e for 10,000 simulations when $\gamma = 1, 2, \ldots, 10$, where $\gamma$ is the proportion of sample size to the number of cells

| $\gamma$ | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Table 1a | 1034 | 3052 | 3471 | 3654 | 3545 | 3467 | 3379 | 3131 | 2962 | 2853 |
| Table 1b | 224  | 245  | 68   | 22   | 4    | 3    | 0    | 0    | 0    | 0    |
| Table 1c | 9    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    |
| Table 5d | 452  | 156  | 51   | 10   | 6    | 0    | 0    | 0    | 0    | 0    |
| Table 5e | 1544 | 1673 | 1657 | 1417 | 1382 | 1051 | 1367 | 617  | 585  | 739  |

Table 7 The 4 × 4 structures of probabilities to generate a multinomial random number

|    | 0.100 | 0.097 | .0002 | 0.102 |
|----|-------|-------|-------|-------|
|    | 0.002 | 0.100 | 0.098 | 0.001 |
|    | 0.095 | .0002 | 0.100 | 0.111 |
|    | .0001 | 0.096 | .0002 | 0.100 |
Table 8  The number of times that the improved estimate is in the outside of the range of Tomizawa et al [24]'s index $\Phi_{1}(\lambda)$ for Table 2a–c, and 7 for 10,000 simulations when $\gamma = 1, 2, \ldots, 10$, where $\gamma$ is the proportion of sample size to the number of cells

|       | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 |
|-------|----|----|----|----|----|----|----|----|----|----|
| Table 2a | 369| 1366| 1752| 1661| 1374| 1160| 944| 705| 581| 438 |
| Table 2b | 31 | 50 | 32 | 8  | 1  | 0  | 0  | 0  | 0  | 0  |
| Table 2c | 0  | 0  | 223| 0  | 97 | 30 | 26 | 0  | 9  | 5  |
| Table 7  | 0  | 0  | 1061| 0   | 1163| 873 | 904| 0  | 840| 1125|

since it is difficult to derive the asymptotic distribution of the improved estimator, the uncertainty quantification of indexes may not be possible. Typically, when the true value of index is on the boundary of its range, it is difficult to quantify the uncertainty using the frequentist approach, such as the plug-in estimator with sample proportions. Our approach is based on the Bayesian approach, and therefore, the uncertainty can be easily quantified using the Monte Carlo method.

Numerical experiments confirmed that our proposed estimator improves the estimation accuracy over the estimator of indexes with the sample proportions in most settings. We also confirmed that the proposed estimator has the same estimation accuracy as the estimator of indexes even in the setting where the contingency tables contain the cells with probabilities close to zero, which is advantageous for the sample proportions. Compared to the improved estimator with only bias correction, our proposed estimator has about the same values of the bias but slightly smaller values of the MSE.

When using the Bayesian estimators of cell probabilities, there is a question of which the Dirichlet parameter to use. We provided one answer, which is to use the Dirichlet parameter that minimizes the MSE of the estimator of indexes in order to improve the accuracy of the estimation of indexes. In fact, numerical experiments showed that when the uniform prior, Jeffreys prior, and the Dirichlet parameter chosen by the Fienberg and Holland [10]'s method are used, their estimation accuracies are considerably worse than that of the estimator with the sample proportions, depending on the probability structure of the contingency tables. In contrast, as mentioned above, our proposed estimator did not become considerably worse than the estimator with the sample proportions, and our estimator maintained stable estimation accuracy in all settings.

Surprisingly, we confirmed that improving the estimator of indexes itself improves the estimation accuracy rather than using the improved estimators of cell probabilities in the estimation of indexes. Fienberg and Holland [10] asymptotically evaluated the MSE of the Bayesian estimators of the cell probabilities and derived the Dirichlet parameter that minimizes the MSE. Namely, they derived

$$\alpha^{FH} = \arg\min_{\alpha} \lim_{n \to \infty} n^2 \text{MSE}[\hat{p}(\alpha)].$$
However, as shown by numerical experiments, in the estimation of indexes, the Dirichlet parameter chosen by the Fienberg and Holland [10]’s method cannot improve the estimation accuracy of indexes in many cases.

In conclusion, when inferring indexes in contingency tables, we recommend the use of our proposed estimator, which can easily evaluate the uncertainty of indexes and improves the estimation accuracy compared to the estimator of indexes with the sample proportions.

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