Outlier Detection in Contingency Tables based on Minimal Patterns

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Abstract

A new technique for the detection of outliers in contingency tables is introduced. Outliers thereby are unexpected cell counts with respect to classical loglinear Poisson models. Subsets of cell counts called minimal patterns are defined, corresponding to non-singular design matrices and leading to potentially uncontaminated maximum-likelihood estimates of the model parameters and thereby the expected cell counts. A criterion to easily produce minimal patterns in the two-way case under independence is derived, based on the analysis of the positions of the chosen cells. A simulation study and a couple of real-data examples are presented to illustrate the performances of the newly developed outlier identification algorithm, and to compare it with other existing methods.

Keywords: Contingency tables; Robustness; Loglinear models; Outliers; Minimal patterns.

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1 Introduction

In every statistical analysis, observations can occur which "appear to be inconsistent with the remainder of that set of data" (Barnett and Lewis, 1994). The same authors also name outliers in contingency tables among little-explored areas, which is up to day still true. For two-way tables outliers have been treated in a couple of research papers in connection with the multinomial model, e.g.,

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by employing residuals and by defining suitable tests based on them in their detection (Simonoff, 1988; Fuchs and Kenett, 1980; Gupta et al, 2007). Approaches for the detection of outliers in higher-dimensional tables with respect to the Poisson model are also found in the literature (e.g. Upton and Guillen, 1995; Kuhnt, 2004).

In the context of contingency tables we deal with outlying cells rather than individual outlying observations contributing to the cell counts. Therefore, the detection of outliers in contingency tables is based on a sample of size one for each cell count, and this fact implies that any detection procedure must be defined with the greatest caution. Additionally, for more than one outlying cell, their position in the table can be crucial with respect to their identification as well as their effect on data analysis methods. This fact has been recognized in the discussion of outlier detection methods and breakdown concepts for contingency tables by Kuhnt (2000, 2010). Also Rapallo (2012) introduces a notion of patterns of outliers in connection with goodness-of-fit tests by applying techniques from algebraic statistics.

In this paper we follow a new approach towards outlier identification in contingency tables. Going back to the general notion of outliers as observations (or, more precisely: cells) deviating from a structure supported by the majority of the data we define so-called minimal patterns. These sets cover more than half of the cells while at the same time containing just enough cells to ensure full rank of the subdesign matrix of a loglinear model. For each pattern the remaining cell counts are candidate outliers. Although the independence model has a major role in the present paper, our technique based on minimal patterns can be applied to any loglinear model. Moreover, finding these minimal patterns is not an easy task, and for the independence model in two-way tables we derive theoretical results on the nature of minimal patterns. Thus, the independence model is used as a leading example. Nevertheless, we discuss also an example on a three-way table under conditional independence in order to show the practical applicability of the notion of minimal pattern under a general loglinear model.

To actually identify the outliers, we suggest two possible algorithms by running through all minimal patterns and using the notion of α -outliers.

The paper is organized as follows. Section 2 briefly recalls α -outliers with respect to loglinear Poisson models and one-step outlier identification methods based on ML- or L_1 -estimators. In Section 3 we define (strictly) minimal patterns and present two outlier detection methods with minimal patterns, called OMP and OMPC, the latter identifying cell counts with the highest count of being an outlier with respect to a minimal pattern. Some results on the connection between mini-

mal patterns and cycles in subtables are derived in Section 4 for the independence model in two-way tables. The performances of the different outlier identification methods are compared by a simulation study in Section 5 and applications to several data sets from the literature are discussed in Section 6. Finally, in Section 7 some conclusions and comments are made.

2 Loglinear Poisson models, estimators and α -outliers

We consider contingency tables with *N* cell counts, assumed to be realizations of random variables Y_j , j = 1,...,N, from a loglinear Poisson model. Any of these models may be presented as generalized linear models (Agresti, 2002) with structural component

$$E(Y_j) = \exp(x'_j\beta) =: m_j, \ j = 1, ..., N$$

where x_j is the j^{th} column of the full rank design matrix $X \in \mathbb{R}^{p \times N}$ of the model and $\beta \in \mathbb{R}^p$ the unknown parameter vector. The maximum likelihood (ML-)estimator of β is given by

$$\widehat{\beta}^{ML} = \underset{\beta \in \mathbb{R}^{p}}{\operatorname{argmax}} \left(\sum_{j=1}^{N} \left(Y_{j} x_{j}^{\prime} \beta - \exp(x_{j}^{\prime} \beta) \right) \right).$$
(1)

A more robust alternative is the L_1 -estimator (Hubert, 1997)

$$\widehat{\beta}^{L_1} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \sum_{j=1}^N |\log Y_j - x'_j \beta|.$$
(2)

Generally, the notion of outliers as surprising observations far away from the bulk of the data has been formalized by so-called α -outlier regions (Davies and Gather, 1993). Thereby observations which are located in a region of the sample space with a very small probability of occurrence with respect to a given model are defined as outliers. A formal definition of outliers in contingency tables is given in Kuhnt (2004):

Definition 1. An observed cell count y_j is called an α -outlier with respect to a loglinear Poisson model if it lies in the outlier region

$$out(\alpha, Poi(m_i)) = \{y \in \mathbb{N} : poi(y, m_i) < K(\alpha)\},\$$

where $poi(\cdot, m_j)$ denotes the probability density function of a Poisson random variable, $\alpha \in (0, 1)$, and $K(\alpha) = \sup\{K > 0 : \sum_{y \in \mathbb{N}} poi(y, m_j) \mathbf{1}_{[0,K]}(poi(y, m_j)) \le \alpha\}$, where $\mathbf{1}_A(x)$ is the indicator function.

The complement of an α -outlier region is called the α -inlier region. All cell counts within an inlier region are named inliers, i.e. inliers are just those observations which are not outliers. Using these notions, one-step outlier identifiers are easily derived, defined next based on the L_1 -estimator. However, the estimator type is exchangeable where robust estimators are of course to be preferred.

Definition 2. Let $\alpha \in (0,1)$ be given. A one-step outlier identifier based on the L_1 -estimator is defined by the following procedure:

- (i) Estimate \hat{m}_j , j = 1, ..., N, for the loglinear Poisson model based on the complete contingency table by the L_1 -estimator.
- (ii) Identify cell counts y_j in α -outlier regions with respect to $Poi(\hat{m}_j)$ as outliers.

The choice of α for the one-step outlier identifiers in relation to the size N of the table is discussed in Kuhnt (2004). This identifier is compared in Section 5 to the new methods developed next.

3 Detecting outliers based on minimal patterns

Consider the notion of outliers as observations which are deviating from a model structure supported by the majority of the data. Here this model is assumed to be a loglinear model characterized by its design matrix X. We look at patterns in the table, given as subsets of the cells, which cover at least half of the table but not more observations than necessary to ensure a full rank design matrix. These patterns are seen as potential core sets of the majority of the data from which individual observations deviate.

Definition 3. Let X be the design matrix of a log-linear model with parameter space \mathbb{R}^p . A subset of cells is called a minimal pattern if

- (*i*) the subset has at least $\left|\frac{N}{2}\right| + 1$ elements;
- *(ii) the corresponding submatrix of X is of full rank;*

(iii) the subset has the minimal number of elements necessary to fulfill condition(i) and condition (ii).

Restricting the considered subset of the cells to those necessary to uniquely define model parameters leads to the definition of strictly minimal patterns.

Definition 4. Let X be the design matrix of a log-linear model with parameter space \mathbb{R}^p . A subset of p cells is called a strictly minimal pattern if the corresponding submatrix of X is of full rank.

If $p = \lfloor \frac{N}{2} \rfloor + 1$ holds, then strictly minimal and minimal patterns coincide. In case of $p < \lfloor \frac{N}{2} \rfloor + 1$, adding $\lfloor \frac{N}{2} \rfloor + 1 - p$ arbitrarily chosen cells to a strictly minimal pattern returns a minimal pattern. Note that not all subsets with *p* cells yield non-singular matrices.

Strictly minimal patterns are different from strictly reconstructable replacement patterns (Kuhnt, 2010). The latter define outlier patterns which are unambiguously identifiable and are used to describe the breakdown behavior of estimators and identification rules. They are closely related and inspired by the notion of unconditionally identifiable interaction patterns in the situation of two-way classification models as introduced by (Terbeck and Davies, 1998).

Before developing algorithms for the detection of outliers based on minimal patterns we fix some notation. Let \mathcal{W} be the set of all W minimal patterns and X the full design matrix in the loglinear Poisson model. Each column of X corresponds to a cell in the contingency table. Taking only the columns of X which correspond to the cells of each minimal pattern yields $X_w, w = 1, ..., W$, and we denote with \mathcal{F}_w the set of column indices in the *w*-th minimal pattern.

A first algorithm on the detection of outliers with minimal patterns called OMP is defined in Algorithm 1 and identifies the set with the minimal number of elements as identified outliers. The idea is that we then have the largest majority of observations well explained by the model given by the minimal pattern.

The idea behind the new outlier detection methods is to run through all minimal patterns and consider each of them as outlier-free subset of the table. The maximum likelihood estimate from these cells provides estimated mean values for all cells. We check for all cell counts outside the pattern if they lie in the α -outlier region with respect to the Poisson distribution given by the estimate. Those cells for which this is true make the set of outliers with respect to the minimal pattern. Hence, we get a set with outliers for each minimal pattern.

Notice that in Algorithm 1 the minimum number of outliers may be attained for more than one minimal pattern. Then more than one solution exist and dif-

Algorithm 1 Outlier detection with minimal patterns (OMP)

for w = 1 to W do $\widehat{\beta}_{w}^{ML} \leftarrow \underset{\beta \in \mathbb{R}^{p}}{\operatorname{argmax}} \left(\sum_{1 \le j \le N \cap j \in \mathscr{F}_{w}} \left(Y_{j} x_{j}' \beta - \exp(x_{j}' \beta) \right) \right)$ for j = 1 to N do Determine $out(\alpha, Poi(\widehat{m}_{j}^{w}))$ for m_{j}^{w} based on $\exp(x_{j}' \widehat{\beta}_{w}^{ML})$ end for $NUMB.OUT_{w} \leftarrow$ Number of outliers for minimal pattern wend for for w = 1 to W do if $NUMB.OUT_{w} = min(NUMB.OUT)$ then Outlier pattern \leftarrow Cells with outliers identified with minimal pattern wend if end for

ferent possible outlier patterns are identified, which can be discussed based on knowledge of the subject.

A slightly different alternative to OMP is implemented in Algorithm 2, called outlier detection with minimal patterns and the count method (OMPC). Here we count how often each cell is identified as outlier with respect to a minimal pattern. If the cell is identified in more than half of the cases it is identified as outlier. We denote the number of minimal patterns not including the cell by r. The choice of the value r/2 as a cut-off in order to discriminate between outliers and inliers is briefly discussed in Section 5.

Algorithm 2 Outlier detection with minimal patterns and the count method (OMPC)

for w = 1 to W do $\widehat{\beta}_{w}^{ML} \leftarrow \underset{\beta \in \mathbb{R}^{p}}{\operatorname{argmax}} \left(\sum_{1 \le j \le N \cap j \in \mathscr{F}_{w}} \left(Y_{j} x'_{j} \beta - \exp(x'_{j} \beta) \right) \right)$ for j = 1 to $N, j \notin \mathscr{F}_{w}$ do Determine $out(\alpha, Poi(\widehat{m}_{j}^{w}))$ for m_{j}^{w} based on $\exp(x'_{j} \widehat{\beta}_{w}^{ML})$ $r_{j} \leftarrow absolute frequency of cell <math>j$ not contained in a minimal pattern if $\#(y_{j} \in out(\alpha, Poi(\widehat{m}_{j}^{w})), j \notin \mathscr{F}_{w}) > r_{j}/2$ then y_{j} is an outlier end if end for When *W* becomes large and the enumeration of all minimal patterns is not feasible, it is possible to introduce a standard Monte Carlo approximation in the algorithms.

As we take the minimal patterns to be potential outlier-free subsets it seems straightforward to employ the ML-estimator. However, the general procedure is open to other choices. Within the simulation study in Section 5 we also use the L_1 -estimator and call the procedure OMPCL1.

Shane and Simonoff (2001) also use elemental subsets of the data to derive robust estimators for categorical data. To detect outliers, we adapt the Pearson least trimmed chi-squared residuals (LTCS) estimator developed by them. In short, Shane and Simonoff create a certain number of elemental subsets and estimate β_{LTCS} for each elemental subset. The subset that minimizes the criterion $\sum_{j=1}^{N} c_j X_{(j)}^2(y_j, \hat{e}_j)$ will be chosen to estimate β_{LTCS} , where

$$c_j = \begin{cases} 1, & \text{if } j \le h \\ 0, & \text{if } j > h, \end{cases}$$

and $X_{(j)}^2$ is the ordered Pearson chi-squared statistic. The authors derive breakdown points for this estimator, which are based on the tuning parameter *h*. The optimal breakdown point of β_{LTCS} is yielded by

$$h = h_{op} \in \left[\lfloor (N+G+1)/2 \rfloor, \lfloor (N+G+2)/2 \rfloor \right],$$

where *G* is the maximum number of linearly independent rows in the design matrix *X*. The generation of elemental subsets can be conducted through minimal patterns, since the authors choose subsets with *p* elements and their design matrices having full rank. They also state that the number of elemental subsets does not have to be very large for their method. In their simulation study, results based on 500 elemental subsets were virtually the same than for 1,000 or 1,500, hence we choose W = 1,000. The algorithm is summarized in the following pseudo-code:

Note that Algorithm 3 can be slightly adjusted to perform outlier detection based on minimal patterns and the LMCS estimator (see Shane and Simonoff, 2001) as well by replacing c_j with $c_h = 1$ and $c_j = 0, j \neq h$. However, simulation results suggest that there is virtually no difference between outlier detection techniques based on LMCS or LTCS, hence we restrict the analyses to the LTCS estimator.

Algorithm 3 Outlier detection with minimal patterns and the LTCS estimator (OLTCS)

$$\begin{split} h &\leftarrow \lfloor (N+G+2)/2 \rfloor \\ c_{j} &\leftarrow \mathbf{1}_{\{j \leq h\}}(j), j = 1, \dots, N. \\ \mathbf{for } w &= 1 \text{ to } 1000 \text{ do} \\ \widehat{\beta}_{w}^{ML} \leftarrow \operatorname*{argmax}_{\beta \in \mathbb{R}^{p}} \left(\sum_{1 \leq j \leq N \cap j \in \mathscr{F}_{w}} \left(Y_{j} x_{j}' \beta - \exp(x_{j}' \beta) \right) \right) \\ \widehat{e}^{w} \leftarrow y - \exp(X \widehat{\beta}_{w}^{ML}) \\ X_{w}^{2} \leftarrow \sum_{1 \leq j \leq N \cap j \in \mathscr{F}_{w}} (y_{j} - \widehat{e}_{j}^{w})^{2} / \widehat{e}_{j}^{w} \\ \mathbf{end for} \\ w^{*} \leftarrow \operatorname{argmin}_{w} \sum_{j=1}^{N} c_{j} X_{w;(j)}^{2} (y_{j}, \widehat{e}_{j}) \\ \mathbf{for } j = 1 \text{ to } N \text{ do} \\ \text{Determine } out(\alpha, Poi(\widehat{m}_{j}^{w^{*}})) \text{ for } m_{j}^{w^{*}} \text{ based on } \exp(x_{j}' \widehat{\beta}_{w^{*}}^{ML}) \\ \mathbf{if } \#(y_{j} \in out(\alpha, Poi(\widehat{m}_{j}^{w^{*}}))) \text{ then} \\ y_{j} \text{ is an outlier} \\ \mathbf{end if} \\ \mathbf{end for} \end{split}$$

4 Minimal patterns and cycles in the independence model

Running through all possible subsets of dimension p to determine the strictly minimal patterns quickly becomes unfeasible for larger dimensional tables. It is therefore important to analyze the structure of these patterns in more detail.

We focus on the loglinear independence model for two-dimensional $I \times J$ contingency tables, assuming without loss of generality $I \leq J$. The design matrix X can be expressed as:

$$X = [a_0, r_1, \dots, r_{I-1}, c_1, \dots, c_{J-1}]',$$
(3)

where a_0 is a unit vector, r_1 is the indicator vector of the first row, c_1 is the indicator vector of the first column, and so on. For instance, the design matrix for 3×3 tables is:

Another classical representation of the same model is given by the design matrix

We use the latter parametrization in our simulation study as it is the usual parametrization implemented in the software for loglinear models, while we use the former parametrization in the proofs, as many formulae become easy to handle.

In this model, the relevant parameter space for the unknown parameter vector β is $\mathbb{R}^{(I+J-1)}$. Table 1 shows that the number of possible patterns with p = I + J - 1 cells as well as the number of (strictly) minimal patterns increases quickly for higher dimensional tables.

| Dimension of the table | 3×3 | 2×5 | 3×4 | 3×5 | 4×4 | 3×6 | 4×5 |
|----------------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| p = I + J - 1 | | | | | | | 8 |
| $\phi = \frac{N}{2} + 1$ | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| $\binom{N}{\phi}$ | 126 | 210 | 792 | 6435 | 11440 | 43758 | 167960 |
| W = # min. patterns | 81 | 80 | 612 | 3780 | 9552 | 26325 | 139660 |
| # str. min. patterns | 81 | 80 | 432 | 2025 | 4096 | 41066 | 105408 |

Table 1: Number of minimal patterns for different independence models

Example 1. *In the case of* 3×3 *tables, the two configurations below have different behavior:*



(the \star 's denote the chosen cells). The configuration on the left hand side produces a singular submatrix, while the configuration on the right hand side produces a non-singular matrix, and hence it is a strictly minimal pattern. At a first glance, we note that in the singular case there is a complete 2×2 subtable among the chosen cells, while in the other case it is not. The relevance of 2×2 subtables in the study of the independence model is well known, see e.g. Agresti (2002), and a different perspective within the field of Algebraic Statistics is investigated in e.g. *Rapallo* (2003). *However, the simple notion of a* 2×2 *submatrix is not sufficient to effectively describe the problem, as shown in the following example:*

| * | * | | |
|---|---|---|---|
| * | | * | |
| | * | * | |
| | | | * |

In this case, the chosen configuration does not contain any 2×2 submatrices, and nevertheless the corresponding submatrix is singular.

To explore the structure of patterns in the table we need to introduce the notion of *k*-cycle.

Definition 5. Let $k \ge 2$. A k-cycle is a set of 2k cells contained in a $k \times k$ subtable, with exactly 2 cells in each row and in each column of the submatrix.

Example 2. In view of Definition 5, a 2-cycle is simply a 2×2 submatrix, while a 3-cycle is a set of 6 cells of the form

| * | * | |
|---|---|---|
| * | | * |
| | * | * |

In case of the independence model, the following theorem shows that the cycles are the key ingredient to check whether a subset of p cells is a strictly minimal pattern.

Theorem 1. A set of p = I + J - 1 cells forms a strictly minimal pattern for the independence model if and only if it does not contain any k-cycles, k = 2, ..., I.

Proof. First, note that a cycle can be decomposed into two subsets of k cells each with one cell in each row and in each column. It is enough to sum the columns of the design matrix X with coefficient +1 for the cells in the first subset and with coefficient -1 for the second subset and we obtain a null vector. Thus, the submatrix is singular and the set does not form a strictly minimal pattern.

Conversely, if the submatrix is singular, then there is a null linear combination among the columns of the submatrix, with coefficients not all zero. Denote with $c_{(i,j)}$ the column of the design matrix corresponding to the cell (i, j). Therefore, we have

$$\gamma_1 c_{(i_1, j_1)} + \ldots + \gamma_p c_{(i_p, j_p)} = 0$$
 (6)

and the coefficients $\gamma_1, \ldots, \gamma_p$ are not all zero. Without loss of generality, suppose that $\gamma_1 > 0$. As the indicator vector of row i_1 belongs to the row span of X and the same holds for the indicator vector of column j_1 , we must have: a cell in the same row $(i_2, j_2) = (i_1, j_2)$ with negative coefficient in Eq. (6); a cell in the same column $(i_3, j_3) = (i_3, j_1)$ with negative coefficient in Eq. (6). Therefore, there must be a cell in row i_3 and a cell in column j_2 with positive coefficients. Now, two cases can happen:

- if the cell (*i*₃, *j*₂) is a chosen cell and its coefficient in Eq. (6) is positive, we have a 2-cycle;
- otherwise, we iterate the same reasoning as above, with another pair of cells.

This shows that there exists a certain number *k* of rows (k > 2), and the same number of columns, with two cells each with a non-zero coefficient. Such cells form by definition a *k*-cycle.

As a corollary, the following algorithm produces strictly minimal patterns:

- 1. Let \mathscr{C} be the set of all cells of the table, and $\mathscr{S} = \emptyset$ the set of the chosen cells.
- 2. For $q \in \{1, \ldots, I+J-1\}$:
 - Choose a cell uniformly from \mathscr{C} , add it to \mathscr{S} , and delete it from \mathscr{C} ;
 - Find all 3-tuples, 5-tuples and so on of cells in \mathscr{S} containing the chosen cell and delete from \mathscr{C} all cells (if any) producing 2-cycles, 3cycles and so on.

Notice that the first three cells are chosen without any restrictions. Moreover, as the algorithm is symmetric on row and column permutation, one has that the strictly minimal pattern is selected uniformly in the set of all strictly minimal patterns.

For 3×3 tables, our statement is equivalent to another criterion, to be found in Kuhnt (2000).

Corollary 1. For the independence model for 3×3 tables, the absence of 2-cycles is equivalent to:

(*i*) no empty rows;

- (*ii*) no empty columns;
- *(iii) for each selected cell, there is at least another cell in the same row or in the same column.*

Proof. Suppose that there is an empty row. In the remaining two rows we have to put 5 cells, and a 2-cycle must appear. The same reasoning holds in the case of an empty column. Finally, if there is a selected cell, say (i, j), with no other cells in the same row or in the same column, we exclude for the remaining 4 cells of the minimal pattern the 5 cells of the *i*-th row and of the *j*-column. Thus the remaining 4 cells are forced to constitute a 2-cycle.

On the other hand, suppose that there is a 2-cycle, and suppose without loss of generality that the cycle is formed by the cells (1,1), (1,2), (2,1), (2,2). The last selected cell can be chosen in 5 different ways. In two cases, (1,3) or (2,3), we have an empty row; in two cases, (3,1) or (3,2), we have an empty column; in the last case, (3,3), this cell has no other cells in the same row or in the same column.

For a general loglinear model, we can define an algorithm to efficiently sample minimal patterns as follows:

- (a) First, choose a strictly minimal pattern.
- (b) Add randomly chosen cells in order to achieve a minimal pattern, if needed.

This procedure can be repeated until every possible minimal pattern has been found. Alternatively, if this is unfeasible due to the dimension of the table, the procedure may be stopped after a certain time or certain number of patterns. In case of the two-way independence model this produces a uniform random minimal pattern, as long as the strictly minimal pattern is uniformly chosen with the algorithm above.

5 Simulation study

In the previous sections we presented different methods to identify α -outliers. To compare different outlier identifiers, Kuhnt (2010) discusses breakdown points of the methods. For the OMPC and the OMP methods, it is not clear if breakdown points or similar criteria can be derived theoretically at all. Hence we present three loglinear Poisson models with varying outlier situations, conduct simulations and

check whether the methods (one-step L_1 (OL1), OLTCS, OMPC and OMPCL1) detect outliers and inliers correctly. We exclude OMP from the comparison as it might lead to results which are not unique and therefore not directly comparable.

We consider three different loglinear Poisson models ((3×3) , (4×4) and (10×10)) and insert various outlying values in the simulated contingency tables. For example, we vary the α -value which determines the outlyingness of the inserted value. For the simulations we adapt the notion of "types" and "antitypes" from Configural Frequency Analysis (von Eye, 2002). A type is defined as a cell in a contingency table with a higher value than the expected cell count, hence above the upper bound of the corresponding α -inlier region. An antitype has a smaller value than the expected cell count of the corresponding α -inlier region.

The six simulated scenarios are described below. The simulations were performed with R (R Development Core Team, 2012) and the results are given in Table 2.

1. We generate 1003×3 contingency tables with $\tilde{X} = \tilde{X}_{3\times 3}$ and $\beta_1 = (4, 0.2, -0.2, 0.4, 0.3)'$ with only one α -outlier ($\alpha = 10^{-4}$) in cell (1,1). Since the position of one outlier in the table is unimportant we place the outlier in the first row and column of each table. The outlier can be seen as a moderate outlier. For the cell (1,1), the outlier region with respect to a Poisson distribution is given by:

$$[0, out_{\text{left}}) \cup (out_{\text{right}}, \infty) = [0, 63) \cup (140, \infty)$$

such that the value 62 is inserted as antitype and 141 as type. Since 3×3 contingency tables have been analyzed in Kuhnt (2000) extensively, we then move to larger tables.

- 2. We generate 100 4 × 4 tables based on $\widetilde{X}_{4\times4}$ created analogous to $\widetilde{X}_{3\times3}$ and $\beta_2 = (3.8, 0.2, -0.2, 0.1, 0.25, 0.3, -0.1)'$. As before, we insert only one moderate α -outlier ($\alpha = 10^{-4}$) in cell (1,1), namely $n_{11} = 39$ as antitype and $n_{11} = 105$ as type.
- 3. Again we generate 100 4 × 4 tables based on β_2 and $\widetilde{X}_{4\times4}$. To see how the methods work with several outliers, we add another α -outlier ($\alpha = 10^{-4}$) resulting in three different situations: Two types, two antitypes, and one type and one antitype. In this scenario, we inserted the outliers in cells (1,1) and (1,2). Notice that the presence of two outliers in the same row can manipulate the estimates of that row in a notably way.

- 4. We reconsider the situation from the third scenario with β_2 and $\widetilde{X}_{4\times 4}$. This time, we replace two values on the main diagonal of the contingency table with α -outliers ($\alpha = 10^{-4}$) in cells (1,1) and (2,2). In this case, the two outliers affect different parameter estimates.
- 5. The last simulation with 4×4 tables based on β_2 and $\widetilde{X}_{4\times 4}$ is similar to the third scenario, but here the outlyingness of the replaced values in cells (1,1) and (1,2) is more extreme. Now, $\alpha = 10^{-8}$ is used.
- 6. We finish the simulation studies with the generation of 100 large 10×10 contingency tables. The corresponding parameter vector is

$$\beta_3 = (3.3, 0.2, -0.2, 0.1, 0.25, 0.3, -0.1, 0.4, 0.2, 0.1, 0.2, -0.4, 0.2, -0.2, 0.1, 0.0, 0.1, -0.3, 0.1)'$$

and the design matrix given by $\tilde{X}_{10\times 10}$. Then α -outliers are inserted in cell (1,1) and cell (2,3), with $\alpha = 10^{-4}$. The number of minimal patterns we consider here is constrained to 500.

All outlier identification methods are always calculated with 0.01-outlier regions of the model given by the parameter estimate. We judge the different methods by the proportion of correctly identified outliers and inliers, given in Table 2. Analyzing the results, some comments are now in order.

- Scenarios 1 and 2 show that the behavior of OL1 is not satisfactory for small tables. The OLTCS procedure has a better sensitivity to outliers while only few inliers are classified wrongly. On the other hand, OMPC has a proportion of correctly classified outliers notably higher than these methods. OMPCL1 is not listed in Scenario 1 because of the exact-fit property of the ML- and L₁-estimator in (3 × 3) tables for minimal patterns, hence both procedure produce the same result.
- Scenarios 3 and 4 prove that the position of the outlying cells within the table is a major issue. In fact, placing the two outliers in the same row, the proportion of correctly classified outliers reduces considerably. This phenomenon is particularly evident in case of two types or two antitypes, since in such cases the outliers give rise to relevant changes in the parameter estimates. With two antitypes in the same row we find again that the OL1 method is almost futile. With respect to Scenario 3, it seems that the OMPC

| Scenario | | | | | | | |
|----------|-----------|-----------------------|---------|-----------------------|------------|----------------|-------------------|
| | | | n_1 | $_1 = 62$ | $n_{11} =$ | 141 | |
| | | estimator | outlie | rs inliers | outliers | inliers | |
| 1 | | OL1 | 0.32 | 0.963 | 0.480 | 0.974 | |
| | | OLTCS | 0.48 | 0.946 | 0.530 | 0.950 | |
| | | OMPC | 0.68 | 0.754 | 0.820 | 0.773 | |
| | | | n_1 | 1 = 39 | $n_{11} =$ | 105 | |
| | | estimator | outlie | rs inliers | outliers | inliers | |
| 2 | | OL1 | 0.62 | 20 0.979 | 0.620 | 0.989 | |
| 2 | | OLTCS | 0.74 | 40 0.943 | 0.680 | 0.937 | |
| | | OMPC | 0.89 | 0.899 | 0.900 | 0.909 | |
| | | OMPCL1 | 0.91 | 0.877 | 0.930 | 0.909 | |
| | | 2 antityp | bes | 1 type, 1 | antitype | 2 t | ypes |
| | ľ | $n_{11} = 39, n_{12}$ | | • • | • • | | $b, n_{12} = 110$ |
| | | | inliers | outliers | inliers | outliers | inliers |
| 3 | OL1 | 0.035 | 0.960 | 0.725 | 0.986 | 0.200 | 0.983 |
| | OLTCS | 0.295 | 0.896 | 0.680 | 0.937 | 0.295 | 0.908 |
| | OMPC | 0.435 | 0.868 | 1.000 | 0.878 | 0.470 | 0.901 |
| | OMPCL1 | 0.615 | 0.833 | 1.000 | 0.846 | 0.720 | 0.874 |
| | | 2 antity | | 1 type, 1 | | 2 ty | pes |
| | | $n_{11} = 39, n$ | - | $n_{11} = 39,$ | • • | $n_{11} = 105$ | - |
| | Estimator | outliers | inliers | outliers | inliers | outliers | inliers |
| 4 | OL1 | 0.740 | 0.976 | 0.495 | 0.980 | 0.635 | 0.984 |
| | OLTCS | 0.795 | 0.948 | 0.670 | 0.923 | 0.695 | 0.921 |
| | OMPC | 0.975 | 0.804 | 0.840 | 0.834 | 0.965 | 0.857 |
| | OMPCL1 | 0.975 | 0.692 | 0.885 | 0.776 | 0.975 | 0.818 |
| | | 2 antityp | | 1 type, 1 | | | ypes |
| | ľ | $n_{11} = 27, n_{12}$ | | $n_{11} = 27, n_{11}$ | • • | | $n_{12} = 128$ |
| | | | inliers | outliers | inliers | outliers | inliers |
| 5 | OL1 | 0.140 | 0.896 | 0.980 | 0.987 | 0.450 | 0.969 |
| _ | OLTCS | 0.370 | 0.870 | 0.835 | 0.936 | 0.430 | 0.898 |
| | OMPC | 0.880 | 0.771 | 1.000 | 0.643 | 0.855 | 0.829 |
| | OMPCL1 | 0.975 | 0.725 | 1.000 | 0.653 | 0.950 | 0.806 |
| | 0 | 2 antit | | 1 type, 1 | | 2 ty | |
| | | $n_{11} = 18,$ | | $n_{11} = 18,$ | J 1 | $n_{11} = 67,$ | |
| | estimator | outliers | inliers | outliers | inliers | outliers | inliers |
| 6 | OL1 | 0.963 | 0.991 | 0.936 | 0.992 | 0.935 | 0.992 |
| U U | OLTCS | 0.850 | 0.929 | 0.855 | 0.933 | 0.815 | 0.932 |
| | OMPC | 0.850 | 0.929 | 0.855 | 0.953 | 1.000 | 0.956 |
| | OMPCL1 | 0.910 | 10.940 | 0.895 | 0.997 | 0.940 | 0.997 |
| | | 0.910 | -9.775 | 0.075 | 0.771 | 0.740 | 0.771 |

Table 2: Proportions of correctly classified outliers and inliers in the 6 simulation scenarios.

method outperforms the OLTCS method concerning outliers in equal directions. On the other hand the inlier detection rate of the OMPC and OMPCL1 method is notably smaller if the outliers are in different rows.

- Comparing scenarios 3 and 5, we observe that all procedures perform better in finding outliers when the outlyingness of the two cells is higher.
- Scenario 6 shows that the proposed methods are still valid for larger tables, even though the differences between the three methods become less relevant. The OMPC outperforms the OLTCS, particularly with regard to outlier detection. Furthermore this is the only scenario where the OMPCL1 has always a smaller outlier detection rate and a higher inlier detection rate than the OMPC method.
- In all simulations the OMPC algorithm is slightly less efficient in detecting inliers. This means that in some few cases it finds more outliers than expected. This issue will be discussed again after the real data examples, in connections with the behavior of the OMP method.

Finally, we need to motivate our choice of $r_j/2$ as the cutoff value in the OMPC algorithm. We considered a simulation study for 3×3 , 4×4 , 5×5 , 6×6 , and 7×7 tables. For each case, we generated 1,000 random contingency tables under two different models:

- M_0 : the null independence model;
- M_1 : the model of independence plus a 10⁻⁴-outlier in the cell (1,1).

For each table, the β vector was chosen with random uniform components on (-0.5, 0.5) except from the first component, fixed at 3.8 in order to control the mean sample size.

Then, we computed the proportion of correct classification of the cell (1, 1) under the two models (i.e., the proportion of outlier detected for M_1 and the proportion of outlier not detected for M_0) running the OMPC algorithm with $\alpha = 0.01$. In order to motivate the choice of the cutoff point, we have computed such proportions for different cutoffs of the form $gr \ (0 < g < 1)$.

The results are displayed in Table 3. The values in Table 3 show that g = 1/2 is a reasonable choice, as it represents the best trade-off between the two types of error.

| | | g = 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 |
|--------------|-------|---------|-------|-------|-------|-------|-------|-------|-------|-------|
| 3×3 | M_0 | 0.984 | 0.976 | 0.950 | 0.898 | 0.828 | 0.752 | 0.650 | 0.498 | 0.450 |
| | M_1 | 0.452 | 0.508 | 0.664 | 0.778 | 0.888 | 0.932 | 0.964 | 0.980 | 0.984 |
| 4×4 | M_0 | 0.998 | 0.988 | 0.984 | 0.956 | 0.894 | 0.844 | 0.746 | 0.608 | 0.418 |
| | M_1 | 0.562 | 0.730 | 0.814 | 0.886 | 0.926 | 0.956 | 0.980 | 0.990 | 0.996 |
| 5×5 | M_0 | 1.000 | 0.998 | 0.990 | 0.964 | 0.926 | 0.868 | 0.768 | 0.644 | 0.462 |
| | M_1 | 0.632 | 0.792 | 0.892 | 0.928 | 0.950 | 0.980 | 0.992 | 0.996 | 1.000 |
| 6×6 | M_0 | 1.000 | 1.000 | 0.990 | 0.984 | 0.956 | 0.936 | 0.880 | 0.786 | 0.588 |
| | M_1 | 0.746 | 0.862 | 0.914 | 0.942 | 0.962 | 0.974 | 0.982 | 0.996 | 0.998 |
| 7×7 | M_0 | 1.000 | 1.000 | 1.000 | 0.994 | 0.980 | 0.952 | 0.912 | 0.814 | 0.654 |
| | M_1 | 0.764 | 0.868 | 0.908 | 0.954 | 0.964 | 0.972 | 0.980 | 0.994 | 0.998 |

Table 3: Proportions of correct classification of cell (1,1) under the models M_0 (where (1,1) is not an outlier) and M_1 (where (1,1) is an outlier)

6 Case studies

We next apply our new outlier detection methods to data sets from the literature. The first data set of artifacts discovered in Nevada is a typical example for outliers from the independence model. The second example of the social mobility of fathers and sons is widely treated in the literature with the general understanding that it actually requires a quasi-independence model, which should become apparent within detecting outliers. The last example on social networks goes beyond two-way tables and shows the applicability of our methods to general loglinear models.

6.1 Artifacts discovered in Nevada

To see how the various outlier identification algorithms work compared to procedures from the literature, we look at the data in Table 4 (Mosteller and Parunak, 2006). This table shows how far away from permanent water certain types of archaeological artifacts have been found.

| | Diste | ance from | permanent v | vater |
|-----------------|--------|-----------|-------------|---------|
| Artifact | Conti- | Within | 0.25 - 0.5 | 0.5 - 1 |
| type | guity | 0.25 mi | mi | mi |
| Drills | 2 | 10 | 4 | 2 |
| Pots | 3 | 8 | 4 | 6 |
| Grinding stones | 13 | 5 | 3 | 9 |
| Point fragments | 20 | 36 | 19 | 20 |

Table 4: Archaeological finds discovered in Nevada, from Mosteller and Parunak (2006).

The OL1 method yields no outliers for $\alpha = 0.001$. This holds also for the OMP method. In contrast, the OMPC method finds two outliers for $\alpha = 0.001$, i.e. cells (3,1) and (3,2). The OLTCS method detects cell (3,1) as outlier, which is also valid for the OMPCL1 method. Looking at the OMPC method with a smaller $\alpha = 0.0005$ we find that only cell (3,1) stays an outlying cell in this method. This dataset has also been studied in Simonoff (1988), where cell (3,1) has been declared as "sure outlier" and cell (3,2) can be seen as a border-line situation.

6.2 Study of social mobility in Britain

As second example, we briefly present the results on an example dataset from Glass and Berent (1954). The status categories of fathers and their sons are put together in a (7×7)-contingency table. Goodman (1971) merges certain classes which yields the 3×3 contingency table in Table 5.

| | | | Son | |
|--------|--------|------|--------|-----|
| | | high | middle | low |
| | high | 588 | 395 | 159 |
| Father | middle | 349 | 714 | 447 |
| | low | 111 | 320 | 411 |

Table 5: Status categories of fathers and sons from Glass and Berent (1954).

Here, OMP identifies the observations n_{11} , n_{22} , n_{33} as outliers. The OMPC as well as the OMPCL1 method identify every cell as an outlier, which seems surprising on the one hand, but on the other hand it is coherent since the underlying independence model is obviously the wrong one. The choice of the model seems to be more important to the OMPC and OMPCL1 methods than to the others. The OMP method yields the only intuitively plausible outlier pattern with the main diagonal. A potential alternative is given by the OL1 and OLTCS methods (n_{11} , n_{13} , n_{31} and n_{33} are outliers), while the OMPC and OMPCL1 offer no satisfying results in this case.

6.3 Social networks

As a final example we consider a model different from independence. McKinley (1973) present a study concerning lay consultation and help-seeking behavior based on eighty-seven working-class families in Aberdeen. We consider a threedimensional table on friendship networks of pregnant woman from this data set. The first variable concerns the frequency of interactions with friends, measured as daily $(X_1 = 1)$, once a week or more $(X_1 = 2)$ and less than once a week $(X_1 = 3)$. The geographic proximity to the friends is covered by variable X_2 with the categories walk $(X_2 = 1)$ and bus $(X_2 = 2)$. The last variable X_3 states whether the woman is pregnant with the first $(X_3 = 2)$ or a further child $(X_3 = 1)$. The data are summarized in Table 6.

The model we consider assumes the conditional dependence between X_1 and

| | | <i>X</i> ₂ : <i>Distance</i> | | | | | | | |
|---------------------------|--------|---|-------|-----------|-------|--|--|--|--|
| | | Wall | k | Bus | | | | | |
| <i>X</i> ₃ : | Parity | Not first | First | Not first | First | | | | |
| V. | Daily | 30 | 6 | 2 | 13 | | | | |
| X ₁ : Freq. | Weekly | 19 | 12 | 16 | 8 | | | | |
| гreq. | Less | 5 | 2 | 10 | 4 | | | | |

Table 6: Data set on social networks from McKinley (1973).

 X_3 given X_2 and has design matrix

| | / 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | \ |
|----------------------------|---------------|----|----|----|---|----|----|----|----|----|----|------------------|---|
| | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | -1 | -1 | -1 | -1 | |
| | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | |
| $\widetilde{\mathbf{v}}$ – | 1 | 1 | -1 | -1 | 1 | 1 | -1 | -1 | 1 | 1 | -1 | $-1 \\ -1 \\ -1$ | |
| $\Lambda =$ | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 | · |
| | 1 | 1 | -1 | -1 | 0 | 0 | 0 | 0 | -1 | -1 | 1 | 1 1 | |
| | 0 | 0 | 0 | 0 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | |
| | $\setminus 1$ | -1 | -1 | 1 | 1 | -1 | -1 | 1 | 1 | -1 | -1 | 1 / | / |

Running the five outlier identification methods, we obtain that with the OL1 method the two extreme values are classified as outliers: $n_{111} = 30$ and $n_{121} = 2$. The OLTCS method yields one outlier in cell n_{121} .

Now we compare the previous results with those yielded by minimal patterns. There are $\binom{12}{8} = 495$ sets with eight elements each and 144 of them fulfill Definition 3. The minimal patterns yield 40 times three outliers, 88 times two outliers and 16 times one outlier. Therefore we look at those cases where the OMP method found only one outlier, more precisely cell n_{121} and cell n_{122} (eight times each). So, this method yields two different solutions.

The OMPC method produces similar results. A cell can be detected as an outlier 48 times at most. The cells $n_{111}, n_{121}, n_{122}$ have been detected 48 times, cells n_{311} and n_{312} have not been detected as outliers, the rest of the cells have been found 24 times, hence 50% of the possible cases. It is conspicuous that a cell is either always an outlier, in 50% of the cases or not at all. This fact holds also for other cell counts and the given model. Furthermore, we are not interested in having 10 outliers and 2 inliers, that's why we declare only the cells $n_{111}, n_{121}, n_{122}$ as outliers. The OMPCL1 method yields the outliers detected by OMPC plus two

| | <i>n</i> ₁₁₁ | <i>n</i> ₁₁₂ | <i>n</i> ₁₂₁ | <i>n</i> ₁₂₂ | <i>n</i> ₂₁₁ | <i>n</i> ₂₁₂ | <i>n</i> ₂₂₁ | <i>n</i> ₂₂₂ | <i>n</i> ₃₁₁ | <i>n</i> ₃₁₂ | <i>n</i> ₃₂₁ | <i>n</i> ₃₂₂ |
|--------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| OL1 | * | | * | | | | | | | | | |
| OLTCS | | | * | | | | | | | | | |
| OMP | | | * | | | | | | | | | |
| OWI | | | | * | | | | | | | | |
| OMPC | * | | * | * | | | | | | | | |
| OMPCL1 | * | * | * | * | | | | | * | | | |

additional outliers in cells n_{112} and n_{311} . The comparison of the results from the four methods are summarized in Table 7.

Table 7: Identification results for the Social Network example.

Upton (1980) and Upton and Guillen (1995) also analyze the given contingency table with regard to outliers. They state that n_{122} should be regarded as an outlier because many pregnant women are still working and get there by bus. There they see their co-workers who are also their friends. This cell has been detected as one of the two solutions of the OMP method, which supports the hypothesis that it works good for a reasonable model and rather small contingency tables. The OMPC method also detected n_{122} as an outlier, but not as the only one.

7 Conclusions

From the simulations and the real data examples, we can now summarize the main features of the outlier detection algorithms considered here.

The OL1 method provides a computationally efficient way to detect outliers in contingency tables, but the OMPC method in most cases outperforms this onestep procedure. Using the OMPCL1 method instead of the OMPC results in an increase of the outlier detection rates in most situations while simultaneously decreasing the inlier detection rates. The OLTCS method can be seen as a compromise between OL1 and OMPC for medium-sized tables w.r.t. detection rates, but for bigger tables it is outperformed by the other procedures. The examples suggest that also the OMP method works better than the OL1 method.

On the other hand, the detection of outliers becomes difficult when there are several outliers in one row or in one column (see the third scenario), and more generally the detection is not easy when the proportion of outliers with respect to the number of cells is high, as shown in the last example. However, in practice we expect to have few outlying cells compared to the dimension of the table. Finally, when the outlyingness is higher (see the fifth scenario), the methods identify more outliers as outliers, but also more inliers as outliers.

Of course, it is worth noting that the experiments performed here are not exhaustive. Several further simulations should be implemented to explore the performances of the minimal patterns algorithms, and to adjust the simulation parameters. In particular, the behavior of our algorithms for large sparse tables, or for tables with zero cell counts, still needs to be explored.

Future work is needed on theoretical results on strictly minimal patterns for higher dimensional loglinear models to allow for the development of efficient algorithms. Additionally, alternative estimation methods might be introduced as well as changes in the procedure.

Some forward procedures to detect outliers in classical regression for example also start from minimal subsets of observations (Riani and Atkinson, 2000), however, without the problem of having to determine them first. Then the one which minimise the median of the ordered squared residuals of the remaining observation is chosen as initial outlier free subset to proceed from. The same approach could also be followed up for contingency tables.

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