A Family of Quasisymmetry Models

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Abstract

We present a one-parameter family of models for square contingency tables that interpolates between the classical quasisymmetry model and its Pearsonian analogue. Algebraically, this corresponds to deformations of toric ideals associated with graphs. Our discussion of the statistical issues centers around maximum likelihood estimation.

1 Introduction

Consider a square contingency table with commensurable row and column classification variables $X$ and $Y$. Such tables can arise from cross-classifying repeated measurements of a categorical response variable. They are common in panel and social mobility studies. One of the most cited examples, taken from Stuart [11], is shown in Table 1. It cross-classifies 7477 female subjects according to the distance vision levels of their right and left eyes.

| Left Eye Grade | best  | second | third | worst |
|----------------|-------|--------|-------|-------|
| best           | 1520  | 266    | 124   | 66    |
| second         | 234   | 1512   | 432   | 78    |
| third          | 117   | 362    | 1772  | 205   |
| worst          | 36    | 82     | 179   | 492   |

Table 1: Cross classification of 7477 women by unaided distance vision of right and left eyes.

The most parsimonious model for such tables is the symmetry (S) model, due to Bowker [3]. While the S model is easy to interpret, it is too restrictive and rarely fits well. An important model that often fits well is the quasi-symmetry (QS) model of Caussinus [4]. Kateri and Papaioannou [6] studied the QS model from the information-theoretic point of view and generalized it to a family of models based on the $\phi$-divergence [9]. In their framework, classical QS is closest to the S model under the Kullback-Leibler divergence. However, by changing the divergence used to measure proximity of distributions, alternative QS models are found. For instance, the Pearsonian divergence yields the Pearsonian QS model. For the data in Table 1, Bishop et al. [2] applied the QS model, while [6] applied the Pearsonian QS model, and here these two lead to estimates of similar fit. However, there are other data sets where only one of them performs well. Our goal is to link these two models. We shall construct a one-parameter family of QS models that connects these two. In this way, more options for data analysis are available. One practical application lies in analyzing and comparing...
independent square tables of the same set-up. For example, consider the same panel study carried out at two independent centers, with one of them being modeled only by the classical QS and the other only by the Pearsonian. In this scenario, the two fitted models are not as comparable as we would like. Our approach furnishes in-between compromise models.

In the framework of algebraic statistics [5, 8], our family interpolates between the two most basic classes of discrete variable models, namely, toric models and linear models [8, §1.2]. Indeed, the QS model is toric, and its Markov basis is well-known, by work of Rapallo [10] and Latuszynski-Trenado [5, §6.2]. The Pearsonian QS model reduces to a linear model, specified by the second factors in (3). Its ML degree is the number of bounded regions in the arrangement of hyperplanes \( \{a_i - a_j = 1\} \), by Varchenko’s formula [8, Theorem 1.5].

This paper is organized as follows. Our parametric family of QS models is introduced in Section 2. In Section 3 we derive the implicit representation of our model by polynomial equations in the cell entries. That section is written in the algebraic language of ideals, and it will be of independent interest to scholars in combinatorial commutative algebra [7, 12].

Maximum likelihood estimation (MLE) and the fit of the model are discussed in Section 4. Section 5 examines a natural submodel given by independence constraints. Section 6 discusses statistical applications and presents computations with concrete data sets. Section 7 follows [6, 9] and offers an information-theoretic characterization in terms of \( \phi \)-divergence.

2 Quasisymmetry Models

We consider models for contingency tables of format \( I \times I \). Probability tables \( p = (p_{ij}) \) are points in the simplex \( \Delta_{I^2-1} \). Here \( p_{ij} \) is the probability that an observation falls in the \((i, j)\) cell. We write \( n = (n_{ij}) \) for the table of observed frequencies. The model of symmetry (S) is

\[
p_{ij} = s_{ij} \quad \text{with parameters } s_{ij} = s_{ji} \quad \text{for } 1 \leq i \leq j \leq I.
\]

Here, and in what follows, the table \((s_{ij})\) is non-negative and its entries sum to 1. Geometrically, the S model is a simplex of dimension \((I + 1)/2 - 1\) inside the ambient probability simplex \( \Delta_{I^2-1} \). The classical QS model can be defined, as a model of divergence from S, by

\[
p_{ij} = s_{ij} \frac{2c_i}{c_i + c_j}, \quad i, j = 1, \ldots, I. \tag{2}
\]

The Pearsonian QS model is defined by the parametrization

\[
p_{ij} = s_{ij}(1 + a_i - a_j), \quad i, j = 1, \ldots, I. \tag{3}
\]

Both models are semialgebraic subsets of dimension \((I + 1)/2 + I - 2\) in the simplex \( \Delta_{I^2-1} \). The S model is the subset obtained respectively for \( c_1 = \cdots = c_I \) in (2) or \( a_1 = \cdots = a_I \) in (3). We here study the following quasisymmetry model \((QS_t)\), where \( t \in [0, 1] \) is a parameter:

\[
p_{ij} = s_{ij} \left( 1 + \frac{(1 + t)(a_i - a_j)}{2 + (1 - t)(a_i + a_j)} \right), \quad i \neq j, \quad i, j = 1, \ldots, I. \tag{4}
\]

In all three models, the matrix entries on the diagonal are set to \( p_{ii} = s_{ii} \) for \( i = 1, \ldots, I \). For \( t = 1 \), the model (4) specializes to the Pearsonian QS model (3). For \( t = 0 \), it specializes
to the QS model \((2)\), if we set \(a_i = c_i - 1\). In order for the \(p_{ij}\) to be probabilities (i.e. to lie in the interval \([0, 1]\)), the parameters \(a_i\) will be assumed to satisfy the restriction
\[
t \cdot \max_i a_i - \min_i a_i \leq 1. \tag{5}
\]
Furthermore, if we change the parameters via
\[
s_{ii} = x_{ii} \quad \text{for } i = j \quad \text{and} \quad s_{ij} = x_{ij} \left(1 + (1 - t) \frac{a_i + a_j}{2}\right) \quad \text{for } i \neq j,
\]
then the model \((\text{QS}_t)\), defined in \((4)\), is rewritten in the simpler form
\[
p_{ij} = x_{ij} (1 + a_i - ta_j), \quad i \neq j, \quad i, j = 1, \ldots, I. \tag{6}
\]
Note that \(x_{i+} = \sum_{j=1}^I x_{ij} = \sum_{j=1}^I x_{ji} = x_{i+}\), since the table \((x_{ij})\) is symmetric. For \(t = 1\), the probabilities defined by \((6)\) satisfy \(\sum_{i=1}^I p_{ij} = 1\) for all \(j\). In order to ensure that \(\sum_{i=1}^I p_{ij} = 1\) for \(t \neq 1\) as well, we use the ‘weighted sum to zero’ constraint
\[
\sum_{i=1}^I (x_{i+} - x_{ii}) a_i = 0. \tag{7}
\]

The expressions \((4)\) and \((6)\) are equivalent. Whether one or the other is preferred is a matter of convenience. Maximum likelihood estimation is easier with \((4)\), since the MLEs of the \(s_{ij}\) are rational functions of the observed frequencies \(n_{ij}\). The estimates of the \(a_i\) depend algebraically on \(n\) and they have to be computed iteratively. In the formulation \((6)\), none of the parameters have estimates that are rational in \(n\). We shall see this in Section 4. On the other hand, for our algebraic analysis of the QS\(_t\) model, it is more convenient to use \((6)\).

**Example 2.1.** Fix \(I = 3\). For any fixed \(t\), the model \((6)\) is a hypersurface in the simplex \(\Delta_8\) of all \(3 \times 3\) probability tables. This hypersurface is the zero set of the cubic polynomial
\[
(1 + t + t^2)(p_{12}p_{23}p_{31} - p_{21}p_{32}p_{13}) + t(p_{12}p_{23}p_{13} + p_{12}p_{32}p_{31} + p_{21}p_{23}p_{31} - p_{12}p_{32}p_{13} - p_{21}p_{23}p_{13} - p_{21}p_{32}p_{31}). \tag{8}
\]
For \(t = 0\), we recover the familiar binomial relation that encodes the cycle of length three \([5, \S 6.2]\). Thus, our family of QS\(_t\) models represents a deformation of that Markov basis:
\[
p_{12}p_{23}p_{31} - p_{21}p_{32}p_{13} + O(t).
\]

The generalization of the relation \((8)\) to higher values of \(I\) will be presented in Section 3. □

Another characteristic model for square tables with commensurable classification variables is the model of *marginal homogeneity* (MH), specified by the equations
\[
p_{i+} = p_{+i}, \quad i, j = 1, \ldots, I. \tag{9}
\]
The model of symmetry S implies MH and QS, i.e. \((2)\) with \(c_1 = \cdots = c_I\). By \([2, \S 8.2.3]\), if the models MH and QS hold simultaneously, then S is implied. In symbols, \(S = \text{MH} \cap \text{QS}\). This identity is important in that it underlines the role of the parameters \(c_i\) in the QS model. These express the contribution of the classification category \(i\) to marginal inhomogeneity. We shall prove next that the same identity holds for our generalized QS\(_t\) model.
Proposition 2.2. For any \( t \in [0,1] \), we have \( S = MH \cap QS_t \).

Proof. It is straightforward to verify that \( S \) implies \( MH \) and \( QS_t \) with \( a_i = 0 \), for all \( i \), which leads to \( p_{ij} = x_{ij} = s_{ij} \), for all \( i, j \). On the other hand, under \( QS_t \) as defined by (6), we have

\[
p_{i+} - p_{+i} = (1 + t) \left( a_i (x_{i+} - x_{ii}) - \sum_{j \neq i} a_j x_{ij} \right), \quad i, j = 1, \ldots, I. \tag{10}
\]

Combining this with \( MH \) as in (9), and setting \( y_i := x_{ii} - x_{i+} \), the equation (10) implies

\[
\sum_{j \neq i} a_j x_{ij} + a_i y_i = 0, \quad i, j = 1, \ldots, I. \tag{11}
\]

This can be written in the matrix form \( \mathbf{B} \mathbf{a} = 0 \), where \( \mathbf{a} = (a_1, \ldots, a_I)' \), \( \mathbf{x} = (x_{ij}) \), and

\[
\mathbf{B} = \mathbf{x} - \text{diag}(\mathbf{x}) = \begin{pmatrix} x_{1I} & \cdots & \hat{\mathbf{B}} & x_{I-1,I} \\ \vdots & \ddots & \hat{\mathbf{B}} & \vdots \\ x_{I1} & \cdots & x_{I-1} & y_I \end{pmatrix}.
\]

The matrix \( \hat{\mathbf{B}} \) is strictly diagonally dominant, provided \( |y_i| = x_{i+} - x_{ii} > \sum_{j \neq i} x_{ij} \). This is ensured if all \( x_{ij} \) are positive, as in Remark 2.3; otherwise a separate argument is needed.

By the Levy-Desplanques Theorem, the matrix \( \hat{\mathbf{B}} \) is invertible and \( \text{rank}(\hat{\mathbf{B}}) = I - 1 \). Hence \( \text{rank}(\mathbf{B}) = I - 1 \), since \( \mathbf{B} \mathbf{1} = 0 \). We verify that \( \mathbf{a} = a \mathbf{1} \) is a solution of \( \mathbf{B} \mathbf{a} = 0 \). For \( t = 1 \), (6) now implies \( p_{ij} = x_{ij} = s_{ij} \), for all \( i, j \). For \( t \neq 1 \), combining (7) with the positivity of \( x_{i+} - x_{ii} \), we get \( a = 0 \). Hence symmetry \( S \) holds and the proof is complete.

Remark 2.3. Contingency tables with structural zeros, i.e., cells of zero probability, are rare. If they exist, they usually have a specific pattern (zero diagonal, triangular table). In our set-up it is realistic to assume that there exists an index \( j \) such that \( p_{ij} > 0 \) for all \( i = 1, \ldots, I \). Thus, without loss of generality, we can assume that \( p_{ii} > 0 \) and thus \( x_{ii} > 0 \) for all \( i = 1, \ldots, I \).

Example 2.4. (\( I = 3 \)) Marginal homogeneity defines a linear space of codimension 2, via

\[
\begin{align*}
p_{11} + p_{12} + p_{13} &= p_{11} + p_{21} + p_{31}, \\
p_{21} + p_{22} + p_{23} &= p_{12} + p_{22} + p_{32}, \\
p_{31} + p_{32} + p_{33} &= p_{13} + p_{23} + p_{33}.
\end{align*}
\]

Inside that space, the cubic (8) factors into a hyperplane, which is the \( S \) model \( \{ p_{12} = p_{21}, \quad p_{13} = p_{32}, \quad p_{23} = p_{32} \} \), and a quadric, which has no points with positive coordinates. \( \diamond \)

In the light of Proposition 2.2, the parameter \( a_i \) of the \( QS_t \) model can be interpreted as the contribution of each category \( i \) to the marginal inhomogeneity. By this we mean the difference of \( a_i \) minus the weighted average of all \( a_i \)’s, seen in parentheses in the identity

\[
p_{i+} - p_{+i} = (1 + t)x_{i+} \left( a_i - \sum_j \frac{x_{ij}}{x_{i+}} a_j \right), \quad i, j = 1, \ldots, I. \tag{12}
\]
3 Implicit Equations

We now examine the quasisymmetry models QS$_t$ through the lens of algebraic statistics [5, 8, 10]. We fix a simple graph $G$ with vertex set $\{1, 2, \ldots, I\}$. Let $I_G$ denote the prime ideal of algebraic relations among the quantities $p_{ij} = x_{ij}(1+a_i-ta_j)$ in (6), where $\{i, j\}$ runs over the set of edges $E(G)$. The ideal $I_G$ lives in the polynomial ring $\mathbb{K}[p_{ij} : \{i, j\} \in E(G)]$. Here we take $\mathbb{K} = \mathbb{Q}[t]$ to be the local ring of formal Laurent series in one unknown $t$. One motivation for deriving $I_G$ is the constrained formulation of the MLE problem in Section 4.

The model in Section 2 corresponds to the complete graph on $I$ nodes, denoted $G = K_I$. In particular, for $I = 3$, the ideal $I_{K_3}$ is the principal ideal generated by the cubic (8). Here we work with arbitrary graphs $G$, so as to allow for sparseness in the models. We disregard the 'weighted sum to 0' constraint (7), as this does not affect the homogeneous relations.

Let $E(G)$ denote the set of oriented edges of $G$. For each edge $\{i, j\}$ in $E(G)$ there are two edges $ij$ and $ji$ in $E(G)$. So we have $|E(G)| = 2|E(G)|$. An orientation of $G$ is the choice of a subset $O \subset E(G)$ such that, for each edge $\{i, j\}$ in $E(G)$, either $ij$ or $ji$ belongs to $O$. An orientation of $G$ is called acyclic if it contains no directed cycle.

Let $C$ denote the undirected $n$-cycle, with $E(C) = \{\{1, 2\}, \{2, 3\}, \ldots, \{n, 1\}\}$. Then $C$ has $2^n$ orientations, shown in Figure 1 for $n = 3$. Precisely two of these orientations are cyclic. These directed cycles are denoted by $o_C$ and $\bar{o}_C$. Their edge sets are $E(o_C) = \{12, 23, \ldots, n1\}$ and $E(\bar{o}_C) = \{21, 32, \ldots, 1n\}$. Any orientation $\delta_C$ of $C$ defines a monomial of degree $n$ via

$$p^\delta_C = \prod_{ij \in E(\delta_C)} p_{ij};$$

and we define the integer $c(\delta_C) = 2|E(o_C) \cap E(\bar{o}_C)| - n$. Note that $c(o_C) = n$ and $c(\bar{o}_C) = -n$.

We associate with the $n$-cycle $C$ the following polynomial of degree $n$ with $2^n$ terms:

$$P^C = \sum_{\delta_C} \text{coeff}(\delta_C) \cdot p^\delta_C. \quad (13)$$

The sum is over all orientations $\delta_C$ of $C$, and the coefficients are the scalars in $\mathbb{K}$ defined by

$$\text{coeff}(\delta_C) = \begin{cases} \frac{c(\delta_C)}{|\delta_C|} \cdot \left(t^{r - \frac{|\delta_C|}{2}} + t^{r + 2 - \frac{|\delta_C|}{2}} + \cdots + t^{r + \frac{|\delta_C| - 2}{2}}\right) & \text{if } n = 2r, \\
\frac{c(\delta_C)}{|\delta_C|} \cdot \left(t^{r - \frac{|\delta_C| - 1}{2}} + t^{r + 1 - \frac{|\delta_C| - 1}{2}} + \cdots + t^{r + \frac{|\delta_C| - 1}{2}}\right) & \text{if } n = 2r - 1. \end{cases}$$

Figure 1: The eight orientations $\delta_1, \delta_2, \ldots, \delta_8$ of $C = K_3$.

**Example 3.1.** We consider the cycle $C = K_3$ of length $n = 3$. It has eight orientations, depicted in Figure 1. The corresponding monomials and their coefficients are as follows:
We need to show that $K$.

Thus, the polynomial $P^C$ defined in (13) is the cubic (8) seen in Example 2.1.

We define the classical $QS$ model on the graph $G$ by the parametrization (2) where $\{i, j\}$ runs over the set $E(G)$ of edges of $G$. We write $T_G$ for the ideal of this model. This is a toric ideal whose Markov basis is obtained from the cycle polynomials $P^C$ by setting $t = 0$:

**Lemma 3.2.** The ideal $T_G$ has a universal Gröbner basis consisting of the binomials

$$P^C|_{t=0} = p^{o(C)} - p^{d(C)}$$

for all cycles $C$ in $G$. (14)

**Proof.** The identity in (14) is straightforward from the definition of $c(\delta_C)$ and $\text{coeff}(\delta_C)$. It was shown in [5, §6.2] that the binomials $p^{o(C)} - p^{d(C)}$ form a Markov basis for $QS$. Since the underlying model matrix is totally unimodular, the Markov basis is also a Graver basis, and hence it is a universal Gröbner basis, by [12, Propositions 4.11 and 8.11].

**Example 3.3.** For $I = 4$ the model $QS_t$ corresponds to the complete graph $K_4$. This graph has seven undirected cycles $C$, four of length 3 and three of length 4. Its defining prime ideal $I_{K_4}$ is generated by four cubics and three quartics, all of the form $P^C$. For $t = 0$, we recover the binomials corresponding to the seven moves that are listed in [10, §5.4, page 395].

This example is explained by the following theorem, which is our main result in Section 3.

**Theorem 3.4.** The prime ideal $I_G$ of the quasisymmetry model associated with an undirected graph $G$ is generated by the cycle polynomials $P^C$ where $C$ runs over all cycles in $G$.

**Proof.** We begin by proving that $P^C$ lies in $I_G$. The image of $P^C$ under the substitution $p_{ij} \mapsto x_{ij}(1 + a_i - ta_j)$ can be written as $Q^C \times \prod_{(i,j) \in E(C)} x_{ij}$, where $Q^C$ is a polynomial in $\mathbb{K}[a_1, \ldots, a_n]$. Since each term $p^{\delta_C}$ of $Q^C$ is divisible by either $p_{1n}$ or $p_{n1}$, we can write

$$Q^C = (1 + a_1 - ta_n)T_{1n} + (1 + a_n - ta_1)T_{n1}.$$ (15)

We need to show that $Q^C$ is zero. To do this, we shall establish the following identities:

$$T_{1n} = (-1)^{|\mathbb{Z}_2|+1}(t+1)^{2r-2}(1+a_n-ta_1)\prod_{i=2}^{n-1}(1+a_i-ta_i)$$

and

$$T_{n1} = (-1)^{|\mathbb{Z}_2|}(t+1)^{2r-2}(1+a_1-ta_n)\prod_{i=2}^{n-1}(1+a_i-ta_i).$$

To prove these, we shall use the decompositions

$$T_{1n} = (1+a_1-ta_2)T_{1n,12} + (1+a_2-ta_1)T_{1n,21}$$

and

$$T_{n1} = (1+a_1-ta_2)T_{n1,12} + (1+a_2-ta_1)T_{n1,21}.$$
(i) $T_{1n,12} = (-1)^{\lfloor \frac{n-2}{2} \rfloor} t(t + 1)^{2r-3}(a_2 - a_n) \prod_{i=3}^{n-1} (1 + a_i - t a_i)$,

(ii) $T_{1n,21} = (-1)^{\lfloor \frac{n-2}{2} \rfloor} (t + 1)^{2r-3}(t^2 a_2 - t - a_n - 1) \prod_{i=3}^{n-1} (1 + a_i - t a_i)$.

Let $C'$ be the cycle 2-3-⋯-n. In analogy to (15), we write

$$Q^{C'} = (1 + a_2 - t a_n) S_{2n} + (1 + a_n - t a_2) S_{2n}.$$

Note that for any orientation $\delta_C$ of $C$ in which $1n$ and 12 belong to $E(\delta_C)$, we have

$$c(\delta_C) = \begin{cases} c(\delta_{C'}) - 1 & \text{if } n2 \in E(\delta_{C'}), \\ c(\delta_{C'}) + 1 & \text{if } 2n \in E(\delta_{C'}). \end{cases}$$

Also note that $\frac{c(\delta_C)}{|c(\delta_C)|} = \frac{c(\delta_{C'})}{|c(\delta_{C'})|}$. In order to prove (i) we consider the following two cases:

**Case 1.** $n$ is an odd number: We claim that $T_{1n,12} = t(S_{n2} + S_{2n})$. Note that $C'$ is an even cycle with $n - 1 = 2(r - 1)$, where $n = 2r - 1$. The coefficient for $\delta_C$ can be written as

$$t \times \frac{c(\delta_C)}{|c(\delta_C)|} \left((t^{r - \frac{|c(\delta_C)|}{2}} - 1 + t^{r - \frac{|c(\delta_C)|}{2}} + \cdots + t^{r + \frac{|c(\delta_C)|}{2} - 2}) + (t^{r - \frac{|c(\delta_C)|}{2}} - 1 + t^{r + 2 - \frac{|c(\delta_C)|}{2}} + \cdots + t^{r + \frac{|c(\delta_C)|}{2} - 3})\right).$$

The first summand corresponds to the orientation $\delta_{C'}$ with $n2 \in E(\delta_{C'})$. The second summand corresponds to the orientation $\delta_{C'}$ with $2n \in E(\delta_{C'})$. By induction on $n$, we have

$$S_{2n} = (-1)^{\lfloor \frac{n-2}{2} \rfloor+1} (t + 1)^{2r-4}(1 + a_n - ta_2) \prod_{i=3}^{n-1} (1 + a_i - t a_i),$$

and

$$S_{n2} = (-1)^{\lfloor \frac{n-2}{2} \rfloor} (t + 1)^{2r-4}(1 + a_2 - ta_n) \prod_{i=3}^{n-1} (1 + a_i - t a_i).$$

Since $-(1 + a_n - ta_2) + (1 + a_2 - ta_n) = (1 + t)(a_2 - a_n)$, the claim (i) holds for $n$ odd.

**Case 2.** $n$ is an even number: We will first show that $T_{1n,12} = t(S_{n2} + S_{2n})/(1 + t)^2$. Here $C'$ is an odd cycle on $n - 1 = 2r - 1$ vertices, where $n = 2r$. The coefficient for $\delta_C$ equals

$$\frac{t}{(1 + t)^2} \times \frac{c(\delta_C)}{|c(\delta_C)|} \left((t^{r - \frac{|c(\delta_C)|}{2}} - 1 + 2t^{r - \frac{|c(\delta_C)|}{2}} + \cdots + 2t^{r + \frac{|c(\delta_C)|}{2} - 1} + t^{r + \frac{|c(\delta_C)|}{2} - 1})\right).$$

This sum can be decomposed as

$$t^{r - \frac{|c(\delta_C)|}{2}} + t^{r - \frac{|c(\delta_C)|}{2}} + \cdots + t^{r + \frac{|c(\delta_C)|}{2} - 1} + t^{r - \frac{|c(\delta_C)|}{2} - 1} + \cdots + t^{r + \frac{|c(\delta_C)|}{2} - 2},$$

where the first summand corresponds to the orientation $\delta_{C'}$ with $n2 \in E(\delta_{C'})$, and the second summand corresponds to the orientation $\delta_{C'}$ with $2n \in E(\delta_{C'})$. Therefore $T_{1n,12} = \frac{t(S_{n2} + S_{2n})}{(1 + t)^2}$.

By induction on $n$, we have

$$S_{2n} = (-1)^{\lfloor \frac{n-2}{2} \rfloor+1} (t + 1)^{2r-2}(1 + a_n - ta_2) \prod_{i=3}^{n-1} (1 + a_i - t a_i)$$

and

$$S_{n2} = (-1)^{\lfloor \frac{n-2}{2} \rfloor} (t + 1)^{2r-2}(1 + a_2 - ta_n) \prod_{i=3}^{n-1} (1 + a_i - t a_i).$$

Since $-(1 + a_n - ta_2) + (1 + a_2 - ta_n) = (1 + t)(a_2 - a_n)$, the result holds for even $n$ as well.
By a similar argument one can prove (ii). Now applying (i) and (ii) and the equality
\[-(1 + a_2 - ta_2)(1 + a_n - ta_1)(1 + t) = (1 + a_1 - ta_2)(a_2 - a_n)t + (1 + a_2 - ta_1)(t^2a_2 - t - a_n - 1),
\]
we obtain
\[T_{1n} = (-1)^{\left\lfloor \frac{n-2}{2} \right\rfloor + 1}(t + 1)^{2r-2}(1 + a_n - ta_1) \prod_{i=2}^{n-1}(1 + a_i - ta_i).\]
The identity for \(T_{1n}\) is analogous. It follows that \(P^C \in \mathcal{I}_G\) for all cycles of \(G\).

It remains to be shown that the \(P^C\) generate the homogeneous ideal \(\mathcal{I}_G\). Recall that, by Lemma 3.2, the images of the \(P^C\) generate this ideal after we tensor, over the local ring \(\mathbb{K}\), with the residue field \(\mathbb{Q} = \mathbb{K}/\langle t \rangle\). Hence, by Nakayama’s Lemma, the \(P^C\) generate \(\mathcal{I}_G\).

**Remark 3.5.** In Theorem 3.4 we can replace the local ring \(\mathbb{K} = \mathbb{Q}[t]\) with the polynomial ring \(\mathbb{Q}[t]\) because no \(t\) appears in the leading forms \((P^C)_{t=0}\). This ensures that \(\mathbb{Q}[t][p_{ij}]\) modulo the ideal \(\langle P^C : C \text{ cycle in } G \rangle\) is torsion-free, hence free, and therefore flat over \(\mathbb{Q}[t]\).

In statistical applications, the quantity \(t\) will always take on a particular real value. In the remainder of this paper, we assume \(t \in \mathbb{R}\), and we identify \(\mathcal{I}_G\) with its image in \(\mathbb{R}[p_{ij}]\).

**Corollary 3.6.** For any \(t \in \mathbb{R}\), the cycle polynomials \(P^C\) generate the ideal \(\mathcal{I}_G\) in \(\mathbb{R}[p_{ij}]\).

Theorem 3.4 furnishes a (flat) degeneration from \(\mathcal{I}_G\) to the toric ideal \(\mathcal{T}_G\). Geometrically, we view this as a degeneration of varieties (or semialgebraic sets) from \(t > 0\) to \(t = 0\). Lemma 3.2 concerns further degenerations from the toric ideal \(\mathcal{T}_G\) to its initial monomial ideals \(\mathcal{M}_G\). Any such \(\mathcal{M}_G\) is squarefree and serves as a combinatorial model for both \(\mathcal{T}_G\) and \(\mathcal{I}_G\).

We describe one particular choice and draw some combinatorial conclusions. Fix a term order on \(\mathbb{R}[p_{ij}]\) with the property that \(p_{ij} \succ p_{k\ell}\) whenever \(i < k\), or \(i = k\) and \(j < \ell\). For any cycle \(C\), we label the two directed orientations \(o_C\) and \(\bar{o}_C\) so that \(p^{o_C} \succ p^{\bar{o}_C}\). Fix a spanning tree \(T\) of \(G\). Let \(P_T\) denote the ideal generated by all unknowns \(p_{ij}\) where \(\{i, j\} \in E(G) \setminus E(T)\) and \(p_{ij}\) divides \(p^{o_C}\), where \(C\) is the unique cycle in \(E(T) \cup \{\{i, j\}\}\). Then
\[\mathcal{M}_G = \text{in}_{\succ} (\mathcal{T}_G) = \langle p^{o_C} : C \text{ cycle in } G \rangle = \bigcap_T P_T,\] where the intersection is over all spanning trees of \(G\). The simplicial complex associated with \(\mathcal{M}_G\) is a regular triangulation of the Lawrence polytope of the graph \(G\). This triangulation is shellable and hence our ideals are Cohen-Macaulay. We record the following information.

**Proposition 3.7.** The ideals \(\mathcal{M}_G, \mathcal{T}_G\) and \(\mathcal{I}_G\) define varieties of dimension \(|E(G)| + 1\) in affine space, and their common degree is the number of spanning trees of the graph \(G\).

**Proof.** Each of the components \(P_T\) in (16) has codimension \(|E(G) \setminus E(T)| = |E(G)| - 1\) in \(G\).

**Example 3.8.** Consider the graph \(G\) depicted in Figure 2. The associated toric ideal equals
\[\mathcal{T}_G = \langle p_{12}p_{23}p_{31}, p_{12}p_{24}p_{11} - p_{21}p_{12}p_{14}, p_{13}p_{32}p_{24}p_{41} - p_{31}p_{23}p_{42}p_{14} \rangle.
\]
This has codimension 2 and degree 8. Its (underlined) initial monomial ideal \(\mathcal{M}_G\) equals
\[\langle p_{12}, p_{13} \rangle \cap \langle p_{12}, p_{32} \rangle \cap \langle p_{12}, p_{24} \rangle \cap \langle p_{12}, p_{41} \rangle \cap \langle p_{23}, p_{41} \rangle \cap \langle p_{23}, p_{24} \rangle \cap \langle p_{21}, p_{31} \rangle \cap \langle p_{31}, p_{41} \rangle.
\]
These primes correspond to the eight spanning trees in Figure 2. The ideal \(\mathcal{I}_G\) has three generators, two cubics with 8 terms and one quartic with 16 terms, as in (13). These are obtained from the Markov basis of \(\mathcal{T}_G\) by adding additional terms that are divisible by \(t\).
Figure 2: A graph $G$ on $I = 4$ nodes and its eight spanning trees $T$

4 Maximum Likelihood Estimation

An $I \times I$ data table $n = (n_{ij})$ can arise either by multinomial sampling or by sampling from $I^2$ independent Poisson distributions, one for each of its cells. In both cases, the log-likelihood function, up to an additive constant, equals

$$\ell_n(p) = \sum_{i=1}^{I} \sum_{j=1}^{I} n_{ij} \cdot \log(p_{ij}).$$  \hspace{1cm} (17)

Maximum likelihood estimation (MLE) is the problem of maximizing $\ell_n$ over all probability tables $p = (p_{ij})$ in the model of interest. Here, this is the quasisymmetry model ($QS_t$), where $t$ is a fixed constant in the interval $[0,1]$. This optimization problem can be expressed in either constrained form or in unconstrained form. The constrained MLE problem is written as

$$\text{Maximize } \ell_n(p) \text{ subject to } p \in V(I_G) \cap \Delta_{I^2 - 1},$$ \hspace{1cm} (18)

where $G = K_I$ is the complete graph on $I$ nodes, and $V(I_G)$ is the zero set of the cycle polynomials $P^C$ constructed in Section 3. The unconstrained MLE problem is written as

$$\text{Maximize } \ell_n(a, s).$$ \hspace{1cm} (19)

The decision variables are the vector $a = (a_1, \ldots, a_I)$ and the symmetric probability matrix $s = (s_{ij})$. The objective function in (19) is obtained by substituting (4) into (17). We shall discuss both formulations, starting with a simple numerical example for the formulation (18).

Example 4.1. Let $I = 3$, $t = 2/3$ and consider the data table

$$n = \begin{bmatrix} 2 & 3 & 5 \\ 11 & 13 & 17 \\ 19 & 23 & 29 \end{bmatrix} \text{ with sample size } n_{++} = 122. \,$$

Our aim is to maximize $\ell_n(p)$ subject to the cubic equation (8) and $p_{11} + p_{12} + \cdots + p_{33} = 1$. Using Lagrange multipliers for these two constraints, we derive the likelihood equations by way of [5, Algorithm 2.29]. These polynomial equations in the nine unknowns $p_{ij}$ have 15 complex solutions. Two of the complex solutions are non-real. Of the 13 real solutions, 12 have at least one negative coordinate. Only one solution lies in the probability simplex $\Delta_8$:

$$\hat{p}_{11} = \frac{1}{61}, \quad \hat{p}_{12} = 0.0286294, \quad \hat{p}_{13} = 0.0376289,$$
$$\hat{p}_{21} = 0.0861247, \quad \hat{p}_{22} = \frac{13}{122}, \quad \hat{p}_{23} = 0.1446119, \quad \hat{p}_{31} = 0.1590924, \quad \hat{p}_{32} = 0.1832569, \quad \hat{p}_{33} = \frac{29}{122}. \hspace{1cm} (20)$$

This is the global maximum of the constrained MLE problem for this instance. \hspace{1cm} ◇
The benefit of the constrained formulation is that we can take advantage of the combinatorial results in Section 3, and we do not have to deal with issues of identifiability and singularities arising from the map (4). On the other hand, most statisticians would prefer the unconstrained formulation because this represents parameter estimation more directly.

To solve the unconstrained MLE problem (19), we take the partial derivations of the objective function \( \ell_n(a, s) \) with respect to all model parameters \( a_i \) and \( s_{ij} \). The resulting system of equations decouples into a system for \( a \) and a system for \( s \). The latter is trivial to solve. Using the requirement that the entries of \( s \) sum to 1, it has the closed form solution

\[
\hat{s}_{ij} = \frac{n_{ij} + n_{ji}}{2n_{++}}, \quad i, j = 1, \ldots, I.
\]

After dividing by \( 1 + t \), the partial derivatives of \( \ell_n(a, s) \) with respect to \( a_1, a_2, \ldots, a_I \) are

\[
\sum_{j^{(1)}=1}^{l} \frac{(1 + a_j - ta_j) [n_{ij} (1 + a_j - ta_j) - n_{ji} (1 + a_i - ta_j)]}{(1 + a_i - ta_j)(1 + a_j - ta_i)[2 + (1 - t)(a_i + a_j)]} \quad \text{for } i = 1, 2, \ldots, I.
\]

This system of equations has infinitely many solutions, because the model \( QS_t \) is not identifiable. The general fiber of the map (4) is a line in \( a \)-space. Hence only \( I - 1 \) of the \( I \) parameters \( a_i \) can be estimated. One way to fix this is to simply add the constraint \( \hat{a}_I = 0 \).

**Example 4.2.** Let us return to the numerical instance in Example 4.1. Here we simply have

\[
\hat{s}_{11} = 1/61, \quad \hat{s}_{12} = 7/122, \quad \hat{s}_{13} = 6/61, \quad \hat{s}_{22} = 13/122, \quad \hat{s}_{23} = 10/61, \quad \hat{s}_{33} = 29/122.
\]

The equations (22) can be solved in a computer algebra system by clearing denominators and then saturating the ideal of numerators with respect to those denominators. As before, there are precisely 15 complex solutions, of which 13 are real. The MLE is given by

\[
\hat{a}_1 = -0.6594884899731861332, \quad \hat{a}_2 = -0.13818331109451658084, \quad \hat{a}_3 = 0.
\]

These are floating point approximations to algebraic numbers of degree 15 over \( \mathbb{Q} \). An exact representation is given by their minimal polynomials. For the first coordinate, this is

\[
62031304a_1^{15} + 2201861910a_1^{14} + 30829909776a_1^{13} + 206135547000a_1^{12} + 528436383696a_1^{11} - 1126661553720a_1^{10} - 9740892273264a_1^9 - 4305524252579a_1^8 + 26533957305582a_1^7 + 88281552626154a_1^6 + 44254830057030a_1^5 - 76332701171853a_1^4 - 83490498412056a_1^3 + 1857597611688a_1^2 + 29825005557312a_1 + 9354112703280 = 0.
\]

With this, the second coordinate \( \hat{a}_2 \) is a certain rational expression in \( \mathbb{Q}(\hat{a}_1) \). By plugging (23) and (24) into (4) with \( t = 2/3 \), we recover the estimated probability table in (20). \( \diamond \)

For larger cases, solutions to the likelihood equations (22) are computed by iterative numerical methods, such as the unidimensional Newton’s method. The updating equations at the \( q \)-th step of this iterative method are

\[
a_i^{(q)} = a_i^{(q-1)} - \frac{\partial \ell_n(a)/\partial a_i}{\partial^2 \ell_n(a)/\partial a_i^2} |_{a = a^{(q-1)}} \quad \text{for } i = 1, \ldots, I - 1, \quad q = 1, 2, \ldots.
\]
We find it convenient to rewrite the first derivatives (22) as
\[
\frac{\partial \ell_n(a)}{\partial a_i} = (1 + t) \sum_{j=1}^I \frac{s_{ij}}{2 + (1 - t)(a_i + a_j)} \left( 1 - \frac{1 - t}{1 + t} c_{ij} \right) \left( \frac{n_{ij}}{p_{ij}} - \frac{n_{ji}}{p_{ji}} \right).
\] (26)

The second derivative equals
\[
\frac{\partial^2 \ell_n(a)}{\partial a_i^2} = -(1 + t) \sum_{j=1}^I \frac{2(1 - t)s_{ij}}{[2 + (1 - t)(a_i + a_j)]^2} \left( 1 - \frac{1 - t}{1 + t} c_{ij} \right) \left( \frac{n_{ij}}{p_{ij}} - \frac{n_{ji}}{p_{ji}} \right) (27)
\]
\[
- (1 + t) \sum_{j \neq i} \frac{(1 + t)s_{ij}^2}{[2 + (1 - t)(a_i + a_j)]^2} \left( 1 - \frac{1 - t}{1 + t} c_{ij} \right)^2 \left( \frac{n_{ij}}{p_{ij}^2} + \frac{n_{ji}}{p_{ji}^2} \right).
\]

Here \(i = 1, \ldots, I - 1\), the \(p_{ij}\) are the expressions in (4), and
\[
c_{ij} = \frac{(1 + t)(a_i - a_j)}{2 + (1 - t)(a_i + a_j)}.\]

We believe that the numerical solution found by this iteration is always the global maximum in (19). This is implied by the following conjecture, which holds for \(t = 0\) and \(t = 1\).

**Conjecture 4.3.** The Hessian \(H(a) = \left( \frac{\partial^2 \ell_n(a)}{\partial a_i \partial a_j} \right)\) is negative definite for all \(a \in \mathbb{R}^I\) with (5).

We verified this conjecture for many examples with \(t \in (0, 1)\). In each case, we ran our iterative algorithm for many starting values, and it always converged to the same solution.

The diagonal entries of the Hessian matrix are given in (27), while the non-diagonal are
\[
\frac{\partial^2 \ell_n(a)}{\partial a_i \partial a_j} = \frac{2(1 - t)^2 s_{ij} c_{ij}}{[2 + (1 - t)(a_i + a_j)]^2} \left( \frac{n_{ij}}{p_{ij}} - \frac{n_{ji}}{p_{ji}} \right) + \frac{(1 + t)^2 s_{ij}^2}{[2 + (1 - t)(a_i + a_j)]^2} \left[ 1 - \left( \frac{1 - t}{1 + t} c_{ij} \right)^2 \right] \left( \frac{n_{ij}}{p_{ij}^2} + \frac{n_{ji}}{p_{ji}^2} \right).\] (28)

In the iterative algorithm described above, we had fixed the last parameter \(a_I\) at zero. This ensures identifiability, and it is done for simplicity. The constraint \(a_I = 0\) defines a reference point for the other parameters \(a_1, \ldots, a_{I-1}\). Under this constraint, (12) leads to
\[
a_i = \frac{1}{1 + t} \left( \frac{p_i - p_{+i}}{x_{i+}} - \frac{p_{+} - p_{+i}}{x_{+}} \right) \quad \text{for} \quad i = 1, \ldots, I - 1.
\]
This means that the contribution of category \(i\) to marginal inhomogeneity is compared to the last category’s contribution. Hence, in view of (12), a reasonable alternative constraint could be \(\sum_{j=1}^{I-1} \frac{n_{ij}}{x_{i+}} a_j = 0\). This constraint calibrates each category’s contribution to marginal inhomogeneity relative to the weighted average of all \(I\) categories.

**Remark 4.4.** The iterative procedure described above for fitting the QS\(_t\) models was implemented by us in R. The algorithm works regardless of whether we impose the restriction \(a_I = 0\) or not. We noticed that when imposing this constraint, the algorithm requires more iterations to converge. The convergence is also affected by the initial values \(a^{(0)}\) we used. A classical choice would be \(a_i = 0\) for all \(i\), as this corresponds to complete symmetry. However, we observed that for \(a^{(0)}\) with coordinates \(\frac{n_{i+} - n_{+i}}{n_{i+} + n_{+i}}, \quad i = 1, \ldots, I\), the convergence is faster.
5 Quasisymmetric Independence

A natural submodel of (1) is the symmetric independence model (SI), which is given by
\[ p_{ij} = s_is_j, \quad i, j = 1, \ldots, I. \] (29)
The \( I \) parameters \( s_i \) are non-negative and sum to 1. The corresponding probability tables \( p = (p_{ij}) \) are symmetric and have rank 1. The models of quasisymmetric independence (QSI\(_t\)) can be defined analogously to the QS\(_t\) models, by measuring departure from (29). Namely, replacing the symmetric probabilities \( s_{ij} \) in (4) by the factored form in (29), we get
\[ p_{ij} = s_is_j \left( 1 + \frac{(1 + t)(a_i - a_j)}{2 + (1 - t)(a_i + a_j)} \right), \quad i \neq j, \quad i, j = 1, \ldots, I. \] (30)

The MLEs of the parameters of the SI model in (29) are
\[ \hat{s}_i = \frac{n_{ii} + n_{ij}}{2n} \text{ for } i = 1, \ldots, I. \] (31)
These are also the MLEs of the \( s_i \) parameters in the QSI\(_t\) model. The likelihood equations for \( a \) are as before, but with \( p_{ij} \)'s in (26) as defined in (29) and (30). Their numerical solution can be computed with the iterative procedure described in Section 4, adjusted accordingly.

Remark 5.1. In Proposition 2.2, if we replace the models S and QS\(_t\) by SI and QSI\(_t\), then an analogous statement holds. Thus, we have SI = MH \( \cap \) QSI\(_t\) for each \( t \in [0, 1] \).

Following the discussion in Section 3, it would be interesting to derive the implicit equations for the model QSI\(_t\). At present, we have a complete solution only for the special case \( t = 1 \). The quasisymmetric independence model QSI\(_1\) is defined by the parametrization
\[ p_{ij} = s_is_j \cdot (1 + a_i - a_j), \quad 1 \leq i, j \leq I. \] (32)
Alternatively, \( \{i, j\} \) could range over the edges of a graph \( G \), as in Section 3. In the following result, whose proof we omit, we restrict ourselves to the case of the complete graph \( K_I \).

Proposition 5.2. The prime ideal of the QSI\(_1\) model in (32) is generated by the following homogeneous quadratic polynomials (for any choices of indices \( i, j, k, \ell \) among \( 1, \ldots, I \)):
- \((p_{ij} + p_{ji})^2 - 4p_{ii}p_{jj}\),
- \(p_{kk}(p_{ij} - p_{ji}) + p_{ki}p_{jk} - p_{ik}p_{kj}\),
- \((p_{ij} - p_{ji})(p_{jk} - p_{kj}) + 4(p_{jji}p_{ki} - p_{ji}p_{kj})\),
- \(p_{ii}(p_{jk} - p_{kj}) + p_{ij}(p_{ki} - p_{ik}) + p_{ik}(p_{jj} - p_{ji})\),
- \(p_{ii}(p_{jk} - p_{kj}) + p_{j\ell}(p_{ki} - p_{ik}) + p_{k\ell}(p_{ij} - p_{ji})\).

The general case where \( t < 1 \) differs from the \( t = 1 \) case in that the prime ideal of QSI\(_1\) is no longer generated by quadrics. Even for \( I = 3 \), a minimal generator of degree 3 is needed:

Example 5.3. Fix \( I = 3 \). For general \( t \in \mathbb{R} \), we consider the model (30) with \( p_{ii} = s_is_i \) for \( i = 1, 2, 3 \). Its ideal is minimally generated by 7 polynomials: 6 quadrics and one cubic. ♦
We next illustrate the new models and their features on some characteristic examples. The goodness-of-fit of a model is tested asymptotically by the likelihood ratio statistic. The associated degrees of freedom for $QS_t$ and $QSI_t$ are $df(QS_t) = (I - 1)(I - 2)/2$ and $df(QSI_t) = (I - 1)^2$, respectively. As we shall see, the models in each family can perform either quite similar or differ significantly, depending on the specific data under consideration.

A case of similar behavior is the classical vision example of Table 1. The model of $QS_t$ ($t = 0$) has been applied on this data often in the literature, while Kateri and Papaioannou [6] applied Pearsonian $QS$. Both models provide a quite similar fit, namely ($G^2 = 7.27076$, $p$-value = 0.06375) for $QS_0$ and ($G^2 = 7.26199$, $p$-value = 0.06340) for $QS_1$. Here, $df = 3$.

The behavior of the $QS_t$ models for $t \in (0, 1)$ is similar. The log-likelihood values vary from $-16388.11444$ ($t = 0$) to $-16388.11006$ ($t = 1$) while the saturated log-likelihood is $-16384.47906$ (see Figure 3, left). Table 2 gives the MLEs of the expected cell frequencies under the $QS_0$, $QS_1$ and $QS_{2/3}$. For $t = 2/3$ we get $G^2 = 7.26234$, with $p$-value = 0.06399.

Examples for which the members of the $QS_t$ family are not of similar performance are the two $3 \times 3$ tables of Kateri and Papaioannou in [6, Tables 3 and 4], displayed in Table 3 (a) and (b). Here, the $QS_0$ and $QS_1$ model differentiate in their fit. In particular, the data in Table 3 (a) are modeled well by $QS_0$ but not by $QS_1$ ($G_0^2 = 0.18572$ and $G_1^2 = 5.29006$), while the opposite holds for Table 3 (b), since $G_0^2 = 6.29035$ and $G_1^2 = 0.29215$.

| Right Eye Grade | best | second | third | worst |
|-----------------|------|--------|-------|-------|
| best            | 1520 | 266    | 124   | 66    |
| second          | 234  | 1512   | 432   | 78    |
| third           | (236.62/ 236.62/ 236.61) | (418.99/ 418.90/ 418.90) | (88.39 / 88.40/ 88.40) | (201.57/ 201.58/ 201.58) |
| worst           | 36   | 82     | 179   | 492   |

Table 2: Unaided distance vision of right and left eyes for 7477 women. Parenthesized values are ML estimates of the expected frequencies under models (a) $QS_0$, (b) $QS_{2/3}$, and (c) $QS_1$. The behavior of the $QS_t$ models for $t \in (0, 1)$ is similar. The log-likelihood values vary from $-16388.11444$ ($t = 0$) to $-16388.11006$ ($t = 1$) while the saturated log-likelihood is $-16384.47906$ (see Figure 3, left). Table 2 gives the MLEs of the expected cell frequencies under the $QS_0$, $QS_1$ and $QS_{2/3}$. For $t = 2/3$ we get $G^2 = 7.26234$, with $p$-value = 0.06399.

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Table 3: Simulated $3 \times 3$ examples of Kateri and Papaioannou [6], generated by the models (a) $QS_0$ and (b) $QS_1$ (their Tables 3 and 4, respectively). A toy example in (c).

|   | 1   | 2   | 3   |
|---|-----|-----|-----|
| (a) | 1 28 | 10 15 |
| (a) | 1 122 | 126 102 |
| (a) | 1 49 | 22 26 |
| (b) | 1 38 | 128 36 |
| (b) | 1 5 119 43 |
| (b) | 1 12 88 31 |
| (c) | 1 28 | 12 25 |
| (c) | 1 122 | 126 102 |
| (c) | 1 49 | 22 26 |

Figure 4: $p$-values for the $G^2$ goodness-of-fit test of $QS_t$ (left) and $QSI_t$ (right) for $t \in [0, 1]$, along with the significance level $\alpha = 0.05$. Data are from Table 3: (a) solid and (b) dashed.

In such situations, the question arises whether some $t$ is appropriate for both data sets. Finding $t$ such that $QS_t$ works for two or more $I \times I$ tables of the same set-up is of special interest in the study of stratified tables. Using the same model on all strata makes parameter estimates among models comparable. This is a major advantage of the proposed family.

Offering models that lie ‘in-between’ the two extreme cases ($t = 0$ and $t = 1$) may lead to a common model, perhaps not performing as well as $QS_0$ and $QS_1$ in each table, but providing a reasonable fit for both tables. To visualize this, Figure 4 (left) shows the $p$-values of the fit of the $QS_t$ models with $t \in [0, 1]$, for Tables 3 (a) and (b), by solid and dashed curves, respectively, along with the significance level of $\alpha = 0.05$. The best fit occurs for $t = 0.14$ (see also Figure 3, right), giving $G^2 = 1.742943 \times 10^{-6}$ ($p$-value=0.9989) while for $t = 0$ and $t = 1$, it is $G^2 = 0.0610$ ($p$-value=0.8049) and $G^2 = 1.1131$ ($p$-value=0.2914), respectively.

In all examples treated so far, the log-likelihood under $QS_t$ was monotone in $t$ (see Figure 3, left, and Figure 5, upper). This is not always the case. For example, for the data in Table 3 (c), the best fit occurs for $t = 0.036$ (see also Figure 3, right), giving $G^2 = 1.742943 \times 10^{-6}$ ($p$-value=0.9989) while for $t = 0$ and $t = 1$, it is $G^2 = 0.0610$ ($p$-value=0.8049) and $G^2 = 1.1131$ ($p$-value=0.2914), respectively.

Applying the quasisymmetric independence models to Tables 3 (a) and (b), we observe
that \( QSI_0 \) fits well on Table 3 (a) but not on (b), while model \( QS_1 \) is of acceptable fit for both data sets. Indeed, we have \( G^2_a(QSI_0) = 1.3600 \) (\( p\)-value=0.8511), \( G^2_b(QSI_0) = 11.8622 \) (\( p\)-value=0.0184), \( G^2_a(QSI_1) = 6.4643 \) (\( p\)-value=0.1671) and \( G^2_b(QSI_1) = 5.8640 \) (\( p\)-value=0.2095). For the performance of the QSI, model for \( t \in [0, 1] \), see Figure 4 (right) and Figure 5 (lower). For \( t = 0.532 \), the \( p\)-value of the fit of the model is equal to 0.1983 for both data sets.

All the examples of this section were worked out with R-functions we developed for fitting the QS, and QSI, models via the unidimensional Newton’s method. The adopted inferential approach is asymptotic. In cases of small sample size, exact inference can be carried out via an algebraic statistical approach based on our results of Section 3.

7 Divergence Measures

The one-parameter family of QS models we proposed, \( QS_t, t \in [0, 1] \), connects the classical QS model (\( t = 0 \)) and the Pearsonian QS model (\( t = 1 \)). These two belong both to a broader class of generalized QS models that are derived using the concept of \( \phi \)-divergence [6, 9]. Measures of divergence quantify the distance between two probability distributions
and play an important role in information theory and statistical inference. The best known divergence measure is the Kullback-Leibler (KL) divergence. However there exist broader classes of divergences. Such a class, including the KL as a special case, is the $\phi$-divergence. In the framework of two-dimensional contingency tables, this class is defined as follows. Let $p = (p_{ij})$ and $q = (q_{ij})$ be two discrete bivariate probability distributions. The $\phi$–divergence between $p$ and $q$ (or Csiszar’s measure of information in $q$ about $p$) is defined by

$$D_\phi(p, q) = \sum_{i,j} q_{ij} \phi(p_{ij}/q_{ij}).$$

(33)

Here $\phi : [0, \infty) \to \mathbb{R}^+$ is a convex function such that $\phi(1) = \phi'(1) = 0$, $0 \cdot \phi(0/0) = 0$, and $0 \cdot \phi(x/0) = x \cdot \lim_{u \to \infty} \phi(u)/u$. For $\phi(u) = u \log(u) - u + 1$ and $\phi(u) = (u-1)^2/2$, the divergence (33) becomes the KL and the Pearson’s divergence, respectively. We adopt Pardo’s notation in [9]. For properties of $\phi$-divergence, as well as a list of well-known divergences belonging to this family, we refer to [9, Section 1.2]. The differential geometric structure of the Riemannian metric induced by such a divergence function is studied by Amari and Cichocki in [1].

The generalized QS models introduced by Kateri and Papaioannou [6], are based on the $\phi$-divergence and are characterized by the fact that each model in this class is the closest model to symmetry $S$, when the distance is measured by the corresponding divergence measure. The classical QS model corresponds to the KL divergence, while the Pearsonian QS to Pearson’s distance. We shall prove in Theorem 7.1 that the other members of the QS_t family, i.e. for $t \in (0, 1)$, are $\phi$-divergence QS models as well, and we identify the corresponding $\phi$ function.

**Theorem 7.1.** Fix $t \in (0, 1)$ and consider the class of models with given row (or column) marginals $p_{i+}$ (or $p_{+i}$) for $i = 1, \ldots, I$, and with given sums $p_{ij} + p_{ji} = 2s_{ij}$ for $i, j = 1, \ldots, I$. In this class, the QS_t model (4) is the closest model to the complete symmetry model $S$ in (1), where ‘closest’ refers the $\phi$-divergence defined by

$$\phi(u) = f_t(u) - f_t(1) - f_t'(1)(u - 1),$$

where $f_t(u) = (u + \frac{2t}{1-t}) \log(u + \frac{2t}{1-t})$.

(34)

**Proof.** We set $F_t(u) = \phi'_t(u) = \log(u + \frac{2t}{1-t}) - \ell_t$, where $\ell_t = \log(1 + \frac{2t}{1-t})$ is just a constant for given $t$. This choice of constant ensures $\phi'_t(1) = 0$. Then the inverse function to $F_t$ is

$$F_t^{-1}(x) = (\frac{-2t}{1-t}) + e^{x+\ell_t}.$$

With this, we can write

$$p_{ij} = s_{ij} F_t^{-1}(\alpha_i + \gamma_{ij}) = s_{ij}(\frac{-2t}{1-t} + e^{\alpha_i + \gamma_{ij} + \ell_t}) = s_{ij}(\frac{-2t}{1-t} + \frac{\beta_i (\frac{2(1+t)}{1-t})}{\beta_i + \beta_j}),$$

where

$$\beta_i = e^{\alpha_i + \ell_t} \quad \text{and} \quad e^{\gamma_{ij}} = \frac{2(1+t)}{e^{\alpha_i + \ell_t} + e^{\alpha_j + \ell_t}}.$$

We next rewrite $p_{ij}$ as

$$p_{ij} = s_{ij}(1 + \frac{-(1+t)}{1-t} + \frac{\beta_i (\frac{2(1+t)}{1-t})}{\beta_i + \beta_j}) = s_{ij}(1 + \frac{(1+t)(\beta_i - \beta_j)}{\beta_i + \beta_j}).$$

Setting $\beta_i = 1+(1-t)a_i$ and $\beta_j = 1+(1-t)a_j$, this identity translates into our parametrization (4). Now the result follows from [6, Theorem 1]. For the probability table $s$ with symmetry $S$, the $\phi$-divergence $D_\phi(p, s)$ is minimized when $p$ is the probability table satisfying QS_t. \qed
The fact that the QSₜ models are φ-divergence QS models implies that they share all the properties of the φ-divergence QS models (see [6]). As far as we know, the φ-divergence for the parametric φₜ function (34) has not been considered so far. Its study can be the subject of further research, ideally connecting information geometry [1] and algebraic statistics [5].

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