THE GEOMETRY OF STATISTICAL MODELS FOR TWO-WAY
CONTINGENCY TABLES WITH FIXED ODDS RATIOS

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Abstract. We study the geometric structure of the statistical models for
two-by-two contingency tables. One or two odds ratios are fixed and the
corresponding models are shown to be a portion of a ruled quadratic surface
or a segment. Some pointers to the general case of two-way contingency tables
are also given and an application to case-control studies is presented.

1. Introduction

A two-way contingency table gives the joint distribution of two random variables
with a finite number of outcomes. If we denote by \( \{0, \ldots, I - 1\} \) and \( \{0, \ldots, J - 1\} \)
the outcomes of \( X_1 \) and \( X_2 \) respectively, the contingency table is represented by a
matrix \( P = (p_{ij}) \), where \( p_{ij} \) is the probability that \( X_1 = i \) and \( X_2 = j \). The table
\( P \) is also called an \( I \times J \) contingency table, in order to emphasize that the variable
\( X_1 \) has \( I \) outcomes and the variable \( X_2 \) has \( J \) outcomes.

In the analysis of contingency tables odds ratios, or cross-product ratios, are
major parameters, and their use in the study of \( 2 \times 2 \) tables goes back to the
1970’s. For an explicit discussion on this approach see, e.g., [Fie80].

For a \( 2 \times 2 \) table of the form:

\[
\begin{pmatrix}
p_{00} & p_{01} \\
p_{10} & p_{11}
\end{pmatrix}
\]

there is only one cross-product ratio, namely:

\[
r = \frac{p_{00}p_{11}}{p_{01}p_{10}}.
\]

In the general \( I \times J \) case, there is one cross-product ratio for each \( 2 \times 2 \) submatrix
of the table. Thus, they have the form

\[
\frac{p_{ij}p_{kh}}{p_{ih}p_{kj}}
\]

for \( 0 \leq i < k \leq I - 1 \) and \( 0 \leq j < h \leq J - 1 \), see [Agr02] Chapter 2]. In this paper
we will consider the cross-product ratio and other ratios naturally defined.

Odds ratios are used in a wide range of applications, and in particular in case-
control studies in pharmaceutical and medical research. Following the theory of
log-linear models, the statistical inference for the odds ratios is made under asymptotic normality, see for example [BFH75]. More recently, some methods for exact
inference have been introduced, see [Agr02] and [Agr01] for details and further
references. For the theory about the Bayesian approach, see [Lin04].

From the point of view of Probability and Mathematical Statistics, different
descriptions of the geometry of the statistical models for contingency tables are
presented in [Col80] Chapter 2], and in [BFH75] Section 2.7], using vector space
theory. An earlier approach to the geometry of contingency tables with fixed cross-product ratio can be found in [FG70]. In the last few years, the introduction of techniques from Commutative Algebra gave a new flavor to the geometrical representation of statistical models, as shown in, e.g., [PRW01a, Chapter 6], [PRW01b], [GHKM01] and [Sla04].

In this paper we use Algebraic and Geometric techniques in order to describe the structure of some models for two-way contingency tables described through odds ratios.

We first consider the case of $2 \times 2$ contingency tables of the form (1) with the constraints $p_{ij} > 0$ for all $i, j = 0, 1$ and $p_{00} + p_{01} + p_{10} + p_{11} = 1$. If we allow some probabilities to be zero, notice that the ratios are either zero or undefined. Thus we restrict the analysis to the strictly positive case.

In a $2 \times 2$ table we consider the three odds ratios:

\[ r_\times = \frac{p_{00}p_{11}}{p_{01}p_{10}}, \]
\[ r_{||} = \frac{p_{00}p_{10}}{p_{01}p_{11}}, \]
\[ r_\|= \frac{p_{00}p_{01}}{p_{10}p_{11}}. \]

The meaning of the three odds ratios above will be fully explained in Section 3.

Let $r_\times = \alpha^2$, $r_{||} = \beta^2$ and $r_\|= \gamma^2$. For further use, it is useful to make explicit the following identities. Considering $r_\|$ and $r_\|=\$, it is easy to check that:

(2) $\beta\gamma = \frac{p_{00}}{p_{11}}$,

and

(3) $\frac{\beta}{\gamma} = \frac{p_{01}}{p_{10}}$.

In Section 2 we study the geometric properties of some statistical models for $2 \times 2$ contingency tables. We consider models obtained by fixing two odds ratios, showing that the model is represented by a segment in the probability simplex and studying the behavior of the third ratio. In particular, an expression for tables with three fixed ratios is derived. We also recover classical results about models with a fixed odds ratio. In Section 3 we give a glimpse of the general situation of $I \times J$ contingency tables. We focus our attention on $2 \times 3$ tables and we present some of the difficulties arising in the general case. An application to case-control studies is presented in Section 4.

2. Odds Ratios

In this section, we use basic geometric techniques to study the $2 \times 2$ tables having two out of the three ratios $r_\times, r_\|$ and $r_\|=\$ fixed.

We consider a $2 \times 2$ matrix as a point in the real affine 4-space $A^4$. In particular, with the notation of Equation (1), the $p_{ij}$’s are coordinates in $A^4$. A $2 \times 2$ table is a matrix in the open probability simplex

\[ \Delta = \left\{ P = (p_{ij}) \in A^4 : \sum p_{ij} = 1, p_{ij} > 0, i,j = 0,1 \right\}. \]

As our goal is to describe odds ratios for tables, we may assume the ratios to be non-zero positive numbers.
Fixed the first two ratios
\[ r_\times = \alpha^2 \quad \text{and} \quad r_\parallel = \beta^2, \]
we want to answer the following question:

Q1: How can we describe the locus of tables having the assigned
two ratios?

and also

Q2: What are the possible values of the third ratio?

These questions were posed in the AIM computational algebraic statistics plenary
lecture by Stephen Fienberg in 2003. In this situation, some interesting comments
about treating questions Q1 and Q2 were also made.

Consider the quadratic hypersurfaces of \( A_4 \):

\[ Q_\alpha : \alpha^2p_{01}p_{10} = p_{00}p_{11} \]

and

\[ Q_\beta : \beta^2p_{01}p_{11} = p_{00}p_{10}. \]

Notice that a matrix in \( Q_\alpha \cap Q_\beta \) is such that \( r_\times = \alpha^2 \) and \( r_\parallel = \beta^2 \) as soon as
the ratios are defined. Hence, to answer the first question, it is en ough to study
\[ Q_\alpha \cap Q_\beta \setminus Z, \]
where \( Z = \{ P = (p_{ij}) \in A^4 : p_{00}p_{01}p_{10}p_{11} = 0 \} \).

We readily see that \( Q_\alpha \cap Q_\beta \) contains the 2-dimensional skew linear spaces
\[ p_{00} = p_{01} = 0 \quad \text{and} \quad p_{10} = p_{11} = 0 \]
and by general facts on quadrics (see [Har92, page 301]) we know t hat there exist
two more 2-dimensional skew linear spaces, \( R \) and \( S \), such that
\[ Q_\alpha \cap Q_\beta = \{ p_{00} = p_{01} = 0 \} \cup \{ p_{10} = p_{11} = 0 \} \cup R \cup S. \]

Manipulating equations we notice that a point in \( Q_\alpha \cap Q_\beta \setminus Z \) is such that
\[ \frac{p_{00}}{p_{01}} = \alpha^2 \frac{p_{10}}{p_{11}} = \beta^2 \frac{p_{11}}{p_{10}}, \]
and
\[ \frac{p_{10}}{p_{11}} = \beta^2 \frac{p_{01}}{p_{00}} = \frac{1}{\alpha^2} \frac{p_{00}}{p_{01}}. \]

Hence, \( R \) and \( S \) lie in the intersection of the two 3-dimensional spaces
\[ (\alpha p_{10} - \beta p_{11})(\alpha p_{10} + \beta p_{11}) = 0 \]
and
\[ (\beta p_{01} - \frac{1}{\alpha} p_{00})(\beta p_{01} + \frac{1}{\alpha} p_{00}) = 0, \]
where \( \alpha \) and \( \beta \) are chosen to be positive. Only two out of the four resulting 2-
dimensional linear spaces lie in both \( Q_\alpha \) and \( Q_\beta \) and these are \( R \) and \( S \):

\[ R : \alpha p_{10} - \beta p_{11} = \beta p_{01} - \frac{1}{\alpha} p_{00} = 0, \]
\[ S : \alpha p_{10} + \beta p_{11} = \beta p_{01} + \frac{1}{\alpha} p_{00} = 0, \]
which have parametric presentations
\[ R = \{ (\beta u, \frac{1}{\alpha} u, \beta v, \alpha v) : u, v \in \mathbb{R} \}, \]
\[ S = \{(\beta u, -\frac{1}{\alpha} u, \beta v, -\alpha v) : u, v \in \mathbb{R}\} . \]

Summing all these facts up, we get

**Proposition 2.1.** Fix the ratios \( r_\times = \alpha^2 \) and \( r_{\parallel} = \beta^2 \). Then, a matrix has the given ratios if and only if it has the form
\[
\begin{pmatrix}
\beta u \\
\beta v \\
\frac{1}{\alpha} u \\
-\alpha v
\end{pmatrix}
\quad \text{or} \quad
\begin{pmatrix}
\beta u \\
\beta v \\
-\frac{1}{\alpha} u \\
-\alpha v
\end{pmatrix}
\]
with \( u, v \) non-zero real parameters.

Finally, we have to intersect \( R \) and \( S \) with the probability simplex. As we can choose \( \alpha \) and \( \beta \) to be positive, we immediately see that \( S \cap \Delta = \emptyset \) (there is always a non-positive coordinate).

To determine \( R \cap \Delta \), notice that \( R \cap \{ \sum p_{ij} = 1 \} \) is obtained by taking
\[
u = \frac{1 - (\beta + \alpha)v}{\beta + \frac{1}{\alpha}}
\]
in the parametric presentation of \( R \). Hence, we get

**Proposition 2.2.** Fix the ratios \( r_\times = \alpha^2 \) and \( r_{\parallel} = \beta^2 \). Then, a table has the given ratios if and only if it has the form
\[
\begin{pmatrix}
\beta v \\
\beta v \\
\frac{1}{\alpha} v \\
\alpha v
\end{pmatrix}
\]
where \( 0 < v < \frac{1}{\alpha + \beta} \).

This answers question Q1: fixed the two ratios, the tables with those ratios describe a segment in the probability simplex.

**Remark 2.3.** In \[^{[BTH75]}\text{Section 2.7}\], a parametric description of the tables with \( r_\times = 1 \) is written in the form
\[
\begin{pmatrix}
st \\
(1 - t)s \\
(1 - s)(1 - t)
\end{pmatrix}
\]
Let us check that our parametrization contains this as a special case. In order to do this, we will compute the marginal sums
\[
\begin{pmatrix}
\beta \left( \frac{1}{\alpha + 1} - v \right) \\
\beta v \\
\frac{1}{\alpha + 1} - v \\
\frac{\beta + 1}{\alpha + 1}
\end{pmatrix}
\]
Hence, the parametrizations in Equations (4) and (5) are just the same, simply let \( t = \frac{1}{\alpha + 1} \) and \( s = 1 - (\beta + 1)v \).

**Remark 2.4.** Suppose to fix \( r_\times \) and to ask for a geometric description of the locus of tables with this ratio. Using Proposition 2.2 we can easily get an answer. For each value of \( r_{\parallel} \) we get a segment of tables, and making \( r_{\parallel} \) to vary this segment describes a portion of a ruled quadratic surface. Notice that, for \( r_\times = 1 \), this is the result contained in \[^{[BTH75]}\text{Section 2.7}\]. In particular, we recall that matrices such that \( r_\times \) is fixed form a so called Segre variety (i.e., in this case, a smooth quadric surface in the projective three space). For more on this see, e.g., \[^{[GSS05]}\].
Answering question Q2 is just a computation, and we see that

\[ r = \frac{1}{\alpha \beta + 1} \left[ 1 - (\beta + \alpha)v \right]^2, \]

where \( r_x = \alpha^2 \) and \( r_{||} = \beta^2 \). Notice that, fixed \( r_x \) and \( r_{||} \), the third ratio can freely vary in \((0, +\infty)\).

Remark 2.5. We expressed \( r_{||} \) as a function \( r_{||}(\alpha, \beta, v) \), and standard computations show that this is an invertible function of \( v \). In particular, we get

\[ v = \frac{1}{\alpha + \beta + (\alpha \beta + 1)r_{||}}. \]

Thus, given \( r_x = \alpha^2 \), \( r_{||} = \beta^2 \) and \( r_{=} \), we have an explicit description of the unique table with these ratios (use Proposition 2.2).

Clearly, completely analogous results hold if we fix the ratios \( r_x \) and \( r_{=} \).

If we fix the ratios \( r_{||} = \beta^2 \), \( r_{=} = \gamma^2 \) and we argue as above, we get the following:

**Proposition 2.6.** Fix the ratios \( r_{||} = \beta^2 \) and \( r_{=} = \gamma^2 \). Then, a table has the given ratios if and only if it has the form

\[
\begin{pmatrix}
\frac{\beta}{\beta \gamma + 1} \left[ 1 - (\beta + \gamma)v \right] & \gamma v \\
\beta v & \frac{1}{\beta \gamma + 1} \left[ 1 - (\beta + \gamma)v \right]
\end{pmatrix},
\]

where \( 0 < v < \frac{1}{\beta + \gamma} \).

Again, a trivial computation yields:

\[ r_x = \left( \frac{\beta}{\beta \gamma + 1} \right)^2 \frac{[1 - (\beta + \gamma)v]^2}{v^2}, \]

and hence, fixed \( r_{=} \) and \( r_{||} \), the third ratio can freely vary in \((0, +\infty)\), see Remark 2.7.

Remark 2.7. In recent literature, there is an increasing attention to the geometrical structure of probability models for contingency tables. In particular, in [Sla04, Chapter 3] the author presents some results about the geometrical characterization of probability models for \( 2 \times 2 \) contingency tables in terms of the cross-product ratio and the conditional distributions. In the same work the connections between the odds ratios and the classical log-linear and ANOVA-type representations of the probability models are clearly stated. We remark that our notation slightly differs from the one used by A. Slavkovic in her Ph.D. dissertation.

In the same direction, in [LWJ04] the graphical visualization of joint, marginal and conditional distributions on the probability simplex for \( 2 \times 2 \) contingency tables is presented.

3. **The \( 2 \times 3 \) Case**

The study of tables with more than two rows and columns would be of great interest, but the complexity of the problem readily increases as we show in the \( 2 \times 3 \) case.

Consider the \( 2 \times 3 \) matrix

\[
\begin{pmatrix}
p_{00} & p_{01} & p_{02} \\
p_{10} & p_{11} & p_{12}
\end{pmatrix}
\]
and define odds ratios as above for each $2 \times 2$ submatrix. We complete our previous notation by adding a superscript to denote the deleted column, e.g.

$$r^{(1)} = \frac{p_{00}p_{02}}{p_{10}p_{12}}.$$ 

Again, we consider a matrix as a point in a real affine space, in this case $\mathbb{A}^6$. Notice that the ratios are well defined for matrices in $\mathbb{A}^6 \setminus Z$, where $Z$ denotes the set of matrices with at least a zero entry.

Relations among the ratios are the cause of the increased complexity of the higher dimensional cases. For example, as we will see, two of the ratios can always be freely fixed. But, as soon as three ratios are considered, constraints come in the picture.

Easy calculations show that the following relations hold:

$$r^{(0)} r^{(2)} = r^{(1)},$$
$$r^{(0)} r^{(2)} = r^{(1)}$$

and also

$$r^{(0)} = r^{(2)} (r^{(1)})^{-1},$$
$$r^{(1)} = r^{(0)} (r^{(1)})^{-1},$$
$$r^{(2)} = r^{(0)} (r^{(1)})^{-1}.$$

These relations, beside producing constraints on the numerical choice of the ratios, lead to a much more complex geometric situation. We illustrate this by exhibiting some explicit examples (worked out with the Computer Algebra systems Singular and CoCoA). As references for the software, see [CoC04] and [GPS01].

More precisely, we fix some of the ratios and we describe the locus of matrices satisfying these relations in

$$\Sigma^o = \{ P = (p_{ij}) \in \mathbb{A}^6 : \sum p_{ij} = 1 \} \setminus Z,$$

i.e. the space of matrices with non-null entries of sum one. For the sake of simplicity, we do not consider the positivity conditions defining the simplex.

In our geometric descriptions, we will slightly abuse terminology, e.g. we will call a line in $\Sigma^o$ a line in $\mathbb{A}^6$ not contained in $Z$; notice that our lines may have some holes (i.e. the points of intersection with $Z$).

We start by considering the easiest case where two of the ratios are fixed. Already at this stage, a dichotomy arises and we have two different situations, as shown in the following examples:

$$r^{(1)} = r^{(2)} = 1$$

or

$$r^{(1)} = r^{(2)} = 1 \text{ or } r^{(1)} = r^{(2)} = 1 \text{ or } r^{(1)} = r^{(2)} = 1 \text{ or } r^{(1)} = r^{(2)} = 1.$$  

The locus of matrices in $\Sigma^o$ satisfying one of conditions (7) is a 3-dimensional variety of degree 4, while condition (8) describes a 3-dimensional variety of degree 3. Roughly speaking, the degree (see [Har92, page 16] and [Sha95, page 41]) is a measure of the complexity of the variety. For a surface in 3-space, for example, the degree bounds the number of intersections with a line and, in a certain sense, measures how the surface is folded.
Next, we try to fix three of the ratios, for example:

\[(8) \quad r^{(0)} = r^{(1)} = r^{(2)} = 1,\]

\[(9) \quad r_{\|}^{(0)} = r_{\|}^{(1)} = r_{\|}^{(2)} = 1,\]

\[(10) \quad r_{\|}^{(0)} = 4, r_{\|}^{(1)} = 3, r_{\|}^{(2)} = 2.\]

The locus of matrices in $\Sigma^\circ$ satisfying one of conditions (8) is the union of two quadratic surfaces, while condition (9) gives a plane. Moreover, if we consider the same ratios but we vary their values, as in (10), the locus of matrices is now described by a single quadratic surface.

Finally, a glimpse of the case of four fixed ratios:

\[(11) \quad r_{\|}^{(0)} = r_{\|}^{(1)} = r_{\|}^{(2)} = 1,\]

\[(12) \quad r_{\|}^{(0)} = r_{\|}^{(1)} = r_{\|}^{(2)} = 1,\]

In both cases, the locus is described by a curve as expected. But, condition (11) produces the union of four lines, while condition (12) is satisfied by a single line in $\Sigma^\circ$.

The Computer Algebra systems \textbf{Singular} and \textbf{CoCoA} were used to compute primary decompositions (giving the irreducible components of the loci) and Hilbert functions (giving the dimension and the degree of the loci).

4. An application. The case-control studies

Two-by-two contingency tables are natural models for a large class of problems known, in medical literature, as case-control studies. Let us consider a table coming, e.g., from the study of a new pharmaceutical product, or clinical test, designed for the detection of a disease. This is an example of a case-control study.

In a case-control study there are two random variables. The first variable $X_1$ encodes the presence (level 1) or absence (level 0) of the disease. The second variable $X_2$ encodes the result of the clinical test (level 1 if positive, level 0 if negative).

The joint variable $(X_1, X_2)$ has 4 outcomes, namely:

\[(0, 0), (0, 1), (1, 0), (1, 1).\]

Its probabilities form a $2 \times 2$ contingency table:

\[
\begin{pmatrix}
p_{00} & p_{01} \\
p_{10} & p_{11}
\end{pmatrix}.
\]

The probabilities $p_{00}$ and $p_{11}$ are called the probability of true negative and of true positive, respectively. They correspond to the cases of correct answer of the clinical test. The probabilities $p_{10}$ and $p_{01}$ are called the probability of false positive and of false negative, respectively. They correspond to the two types of error which can show in a case-control study. For example, the probability of false negative is the probability that a diseased subject is incorrectly classified as not diseased.

A perfect clinical test which correctly classifies all the subjects would have $p_{01}$ and $p_{10}$ as low as possible, implying a large value of the odds ratio $r_x$. Therefore, the odds ratio $r_x$ measures the validity of the clinical test. In particular, when
The random variables are statistically independent. In our framework this means that, when \( r = 1 \), the result of the clinical test is independent from the presence or absence of the disease. Unless one obtains a large value of \( r \), the clinical test is judged as non efficient. The odds ratio \( r \) is also called Diagnostic Odds Ratio (DOR) in medical literature.

In such a case-control study, two essential indices are the specificity and the sensitivity, defined as:

\[
specificity = \frac{p_{00}}{p_{00} + p_{01}}
\]

and

\[
sensitivity = \frac{p_{11}}{p_{10} + p_{11}}.
\]

Specificity is the proportion of true negative among the diseased subjects, while sensitivity is the proportion of true positive among the non-diseased subjects.

Straightforward computations show that

\[
r = \frac{specificity/(1 - specificity)}{(1 - sensitivity)/sensitivity}.
\]

In view of the definition above, it is easy to show that the relative magnitude of the sensitivity and specificity is measured by the odds ratio \( r \). In fact one can show that

\[
sensitivity/(1 - sensitivity) = \frac{1}{specificity/(1 - specificity)}.
\]

The ratio above is called Error Odds Ratio (EOR).

In recent literature, the DOR and the EOR are relevant parameters for the assessment of the validity of a clinical test. They have received increasing attention in the last few years and a huge amount of literature has been produced. Hence, we refrain from any tentative description and refer the interested reader to, for example, [Kno01].

The meaning of the third ratio \( r \) is not straightforward as explained in [BFH75, Page 21]. However its statistical meaning can be derived using Equations (2) and (3) shown in Section 1.

Finally, we remark that the geometrical structure of the statistical models for case-control studies is very simple. From the results in Section 2 one readily sees that the models are segments or portions of ruled quadratic surfaces. Moreover, from a Bayesian point of view, Propositions 2.2 and 2.6 allow to compute the exact range of the free odds ratio.

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