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# AN ITERATIVE PROCEDURE FOR ESTIMATION IN CONTINGENCY TABLES[1]

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**0. Summary.** Deming and Stephan (1940) first proposed the use of an iterative proportional fitting procedure to estimate cell probabilities in a contingency table subject to certain marginal constraints. In this paper we first relate this procedure to a variety of sources and a variety of statistical problems. We then describe the procedure geometrically for two-way contingency tables using the concepts presented in Fienberg (1968). This geometrical description leads to a rather simple proof of the convergence of the iterative procedure. We conclude the paper with a discussion of extensions to multi-dimensional tables and to tables with some zero entries.

**1. The method.** The iterative proportional fitting procedure (IPFP) was first examined by Deming and Stephan (1940) as a method for estimating cell probabilities, $p_{ij}$, in an $r \times c$ table based on observations, where the marginal totals

(1.1) $$p_{i\cdot} = \sum_{j=1}^{c} p_{ij} \qquad (i = 1, 2, \cdots, r)$$

(1.2) $$p_{\cdot j} = \sum_{i=1}^{r} p_{ij} \qquad (j = 1, 2, \cdots, c)$$

are known and fixed. They proposed the IPFP as a way of arriving at estimates which minimized

(1.3) $$\sum_{i=1}^{r} \sum_{j=1}^{c} (n_{ij} - np_{ij})^2 / n_{ij}$$

subject to the marginal totals, assuming $n_{ij} > 0$.

Stephan (1942) later showed that although the solution provided by the IPFP satisfied the marginal restrictions, it did not satisfy the normal equations and hence was only an approximation to the actual solution. He also pointed out that he had been unable to find a proof of convergence for the IPFP.

Deming (1943), Smith (1947), El-Badry and Stephan (1955), and Friedlander (1961) continued to examine the problem of Deming and Stephan, but they did not provide a proof of the convergence of the IPFP.

The Deming and Stephan IPFP runs as follows:

1. Suppose that there are $n_{ij}$ observations in the $(i, j)$ cell, where

(1.4) $$\sum_{i=1}^{r} \sum_{j=1}^{c} n_{ij} = n,$$

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and we take as our initial values

$$p_{ij}^{(0)} = n_{ij}/n \qquad \forall\, i, j. \tag{1.5}$$

2. At the $(2m)$th step ($m \geqq 1$) we take

$$p_{ij}^{(2m-1)} = p_{ij}^{(2m-2)} \frac{p_{i\cdot}}{p_{i\cdot}^{(2m-2)}} \qquad \forall\, i, j. \tag{1.6}$$

3. At the $(2m+1)$th step we take

$$p_{ij}^{(2m)} = p_{ij}^{(2m-1)} \frac{p_{\cdot j}}{p_{\cdot j}^{(2m-1)}} \qquad \forall\, i, j.$$

4. The iteration is continued until two successive sets of values for the cell probabilities agree sufficiently well.

In Sections 4 and 5 we show that, as $N \to \infty$,

$$p_{ij}^{(N)} \to p_{ij} \qquad \forall\, i, j, \tag{1.8}$$

where the $p_{ij}$ satisfy (1.1) and (1.2).

Mosteller (1968) pointed out that the IPFP can be used for adjusting a table to given marginal totals while preserving the interaction structure of the original table as defined by the crossproduct ratios

$$\frac{n_{ij}\, n_{hk}}{n_{ik}\, n_{hj}} \qquad (i \neq h, j \neq k). \tag{1.9}$$

We first note that $p_{ij}^{(N)}$, for all $N$, is of the form

$$p_{ij}^{(N)} = a_i^{(N)}\, b_j^{(N)} (n_{ij}/n) \qquad \forall\, i, j \tag{1.10}$$

where $a_i^{(N)}$ and $b_j^{(N)}$ are greater than zero. Thus the values $p_{ij}^{(N)}$ at each stage of the iteration satisfy

$$\frac{n_{ij}\, n_{hk}}{n_{ik}\, n_{hj}} = \frac{p_{ij}^{(N)} p_{hk}^{(N)}}{p_{ik}^{(N)} p_{hj}^{(N)}} \qquad (i \neq h, j \neq k). \tag{1.11}$$

The fact that the IPFP does preserve crossproduct ratios allows us to explore the geometrical description of procedure using the concepts presented in Fienberg and Gilbert (1970) and Fienberg (1968), and thus leads to our proof of convergence.

Extensions of the iterative proportional fitting procedure (a) to multidimensional tables and (b) to tables with some $n_{ij} = 0$ are discussed in Section 6.

**2. Uses of the iterative proportional fitting procedure.** Although the IPFP does not provide the correct solution for the problem of Deming and Stephan, it can be used to provide solutions for a wide variety of related problems. We have already discussed how Mosteller (1968) has used the IPFP to adjust a table to given marginal totals while preserving the interaction structure. Other authors, many of whom were not familiar with the work of Deming and Stephan, have also made use of the IPFP and have discussed its properties.

Brown (1959), using an approach described by Lewis (1959), showed that when the IPFP is used to provide cell estimates for a $2 \times 2 \times \cdots \times 2$ table where certain marginal restrictions must be satisfied, the approximation improves at each step of the iteration, according to a minimum information criterion.

Bishop (1967), using a duality theorem of Good (1963, 1965) which gives a relationship between maximum likelihood estimation and maximum entropy (or minimum discrimination information) estimation for contingency tables, first showed that Brown's proof of convergence can be extended to any multidimensional table. She then showed that the IPFP could thus be used to derive maximum likelihood estimates for a variety of loglinear models suggested by Birch (1963). Birch had proved that, for these loglinear models, certain sets of sample marginal totals were the sufficient statistics. Thus the M.L.E.'s had simply to satisfy the marginal restrictions given by the sufficient statistics, and the IPFP could then be used to produce the appropriate estimates. Because of various aspects of the Birch–Bishop models, when the IPFP is used to derive the M.L.E.'s, the initial values in each cell are taken to be equal instead of being given by the observed cell counts as in (1.5). Thus the requirement that all the observed cell counts be positive can clearly be relaxed. Darroch (1962) first suggested the use of the IPFP in this context, and Caussinus (1965) related Darroch's work to that of Deming and Stephan.

Working independently of Bishop, Ireland and Kullback (1968) also showed that Brown's proof of convergence could be extended, and they gave a more rigorous derivation of the convergence. Good (1965, page 75) had previously recognized that Brown's result could be extended in this way, while Dempster (1969) simplified the proof of Ireland and Kullback, and extended the IPFP to deal with problems involving general exponential family models.

Thionet (1961, 1963, 1964) examined the IPFP as the solution to a linear programming problem, similar to those examined by econometricians. He suggested that the convergence of the procedure could be demonstrated by invoking the Brower fixed-point theorem, but his method was somewhat different than the one discussed in this paper. Caussinus (1965), who used the IPFP for contingency table problems, also gave a detailed proof of convergence based on a second method suggested by Thionet. Both Thionet and Caussinus discussed extensions for situations where some of the initial values, $n_{ij}$, are zero. Indeed Caussinus demonstrated convergence when exactly one $n_{ij}$ is zero.

Sinkhorn (1964) showed that corresponding to each positive square matrix $\mathbf{A}$ there is a unique doubly stochastic matrix of the form $\mathbf{D}_1\mathbf{A}\mathbf{D}_2$ where $\mathbf{D}_1$ and $\mathbf{D}_2$ are diagonal matrices with positive main diagonals. He also showed that this doubly stochastic matrix could be obtained as a limit of the iterative process of alternately normalizing the rows and columns of $\mathbf{A}$. In Sinkhorn (1967) the proof was generalized to demonstrate diagonal equivalence to positive rectangular matrices with prescribed rows and columns. Of course, the iterative procedure used to obtain this more general equivalence was simply the IPFP. Menon (1967) gave a simple proof of Sinkhorn's result using a version of the Brower fixed-point theorem. Brualdi, Parter, Schneider (1966), and Sinkhorn and Knopp (1966) deduced

Sinkhorn's first result when **A** is a nonnegative fully indecomposable matrix. Marshall and Olkin (1968) also proved this latter result and suggested the use of an iterative procedure different than the IPFP.

**3. A geometrical interpretation of the iteration.** Fienberg and Gilbert (1970) examined ideas about $2 \times 2$ contingency tables in terms of the geometry of the 3-dimensional simplex. They chose the tetrahedron of reference so that $A_1 = (1, 0, 0, 0)$, $A_2 = (0, 1, 0, 0)$, $A_3 = (0, 0, 1, 0)$, and $A_4 = (0, 0, 0, 1)$ correspond respectively to the tables

(3.1)

| | |
|---|---|
| 1 | 0 |
| 0 | 0 |

| | |
|---|---|
| 0 | 1 |
| 0 | 0 |

| | |
|---|---|
| 0 | 0 |
| 1 | 0 |

| | |
|---|---|
| 0 | 0 |
| 0 | 1 |

The general point $P = (p_{11}, p_{12}, p_{21}, p_{22})$ then corresponds to the table with probabilities, $p_{ij}$, in the $(i, j)$ cells. They then showed that for a given value of the crossproduct ratio

$$\alpha = \frac{p_{11} p_{22}}{p_{12} p_{21}}, \tag{3.2}$$

where $\infty > \alpha > 0$, there exists a doubly ruled *surface of constant* $\alpha$ consisting of points which correspond to all tables having the given crossproduct ratio. One family of rulings consists of lines $TT^*$ with the point $T$ on the line $A_1A_2$ and the point $T^*$ on the line $A_3A_4$ such that

$$\frac{\overline{TA_2}}{\overline{A_1T}} = \frac{t}{1-t} = \alpha \frac{\overline{T^*A_4}}{\overline{A_3T^*}} \qquad 0 \leqq t \leqq 1, \tag{3.3}$$

while the other family of rulings consists of lines $SS^*$ with $S$ on $A_1A_3$ and $S^*$ on $A_2A_4$ such that

$$\frac{\overline{SA_3}}{\overline{A_1S}} = \frac{s}{1-s} = \alpha \frac{\overline{S^*A_4}}{\overline{A_2S^*}} \qquad 0 \leqq s \leqq 1. \tag{3.4}$$

Figure 3.1 shows the surface for $\alpha = 1$, when the corresponding tables have rows and columns which are independent. Figure 3.2 shows the surface corresponding to $\alpha = 3$.

As we noted in Section 1, $\alpha$ remains invariant under row and column multiplication, and thus the tables produced at each step of the IPFP have the same value of $\alpha$ as the original table. The points corresponding to the tables at each step of the iteration thus lie on a particular *surface of constant* $\alpha$. We can easily show that the $(2m)$th step of the IPFP corresponds to moving from the point produced at the $(2m-1)$th step to a new point along one of the family of rulings, $\{TT^*\}$, while the $(2m+1)$th step corresponds to moving from the point produced at the $(2m)$th step to a new point along one of family of rulings, $\{SS^*\}$.

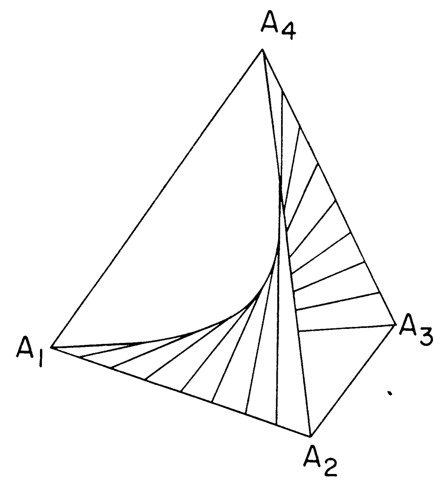


FIG. 3.1. The surface of independence defined by the family of lines $TT^*$.

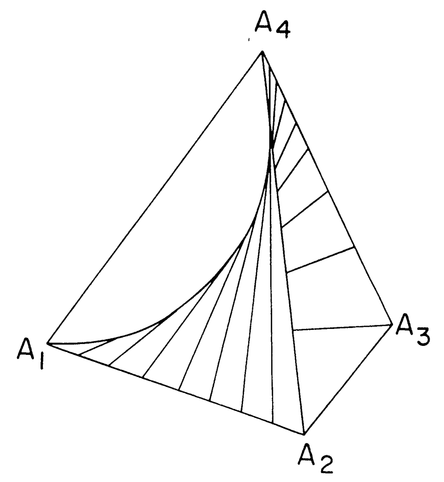


FIG. 3.2. The surface of constant $\alpha$ ($\alpha = 3$) defined by the family of lines $TT^*$.

Fienberg (1968) examined ideas about $r \times c$ tables in terms of the geometry of the $(rc-1)$-dimensional simplex,

$$S_{rc} = \{(x_{11}, x_{12}, \cdots, x_{1c}; \cdots; x_{r1}, \cdots x_{rc}) : x_{ij} \geqq 0, \textstyle\sum_i \sum_j x_{ij} = 1\}. \tag{3.5}$$

Generalizing the results of Fienberg and Gilbert, he showed that the locus of all points corresponding to tables with a given set of crossproduct ratios is a *manifold of constant interaction* generated by a family of non-intersecting $(c-1)$-flats, and by a family of non-intersecting $(r-1)$-flats. Each of the generating $(c-1)$-flats meets each of the generating $(r-1)$-flats in exactly one point. These manifolds are special cases of the determinantal manifolds discussed by Room (1938).

Since the crossproduct ratios remain constant at each step of the IPFP (see (1.11)), all the points corresponding to the tables produced at each step of the iteration thus lie on a particular *manifold of constant interaction*. Again, we can easily show that the $(2m)$th step of the IPFP corresponds to moving from the point produced at the $(2m-1)$th step to a new point along one of the generating $(c-1)$-flats, while the $(2m+1)$th step corresponds to moving from the point produced at the $(2m)$th step to a new point along one of the generating $(r-1)$-flats.

**4. Convergence of the IPFP for 2 × 2 tables.** First we must determine the crossproduct ratio $\alpha_0$ for the given table. If $\alpha_0 = 1$, the rows and columns of the table are said to be independent, and the iteration obviously converges by the end of the first cycle (i.e., by the end of the 3rd step).

If $\alpha_0 \neq 1$, we map the *surface of constant* $\alpha_0$ onto the unit square, $U$, so that

$$A_1A_2,\ A_2A_4,\ A_4A_3 \quad \text{and} \quad A_3A_1$$

are mapped into the sides of $U$ as in Figure 4.1, while preserving both distances between points on each of these lines and incidences between generators. This mapping is a homeomorphism, and so we need only show convergence in the Euclidean metric on $U$. Furthermore, without loss of generality we may assume

$$p_{1\cdot} = p_{2\cdot} = p_{\cdot 1} = p_{\cdot 2} = \tfrac{1}{2}, \tag{4.1}$$

for otherwise the mapping onto $U$ can be redefined to make distances between points on the sides correspond to the situation where (4.1) is true.

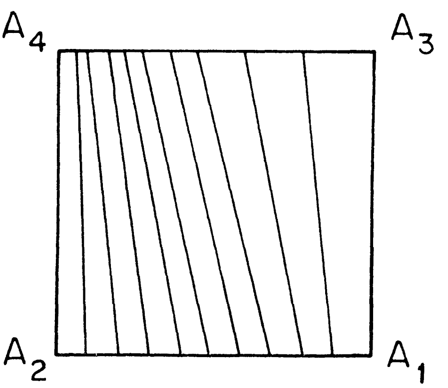


FIG. 4.1. The mapping of the surface of constant $\alpha$ ($\alpha = 3$), with the family of lines $TT^*$, into the unit square.

As an illustration, Figure 4.2 shows the course of successive iterations for a particular $\alpha_0$ and starting point. Note that the starting point must always be in the interior of $U$ since $n_{ij} > 0\ \forall i, j$.

The proof of convergence now rests on the following observation: Each generator of the family $\{TT^*\}$ makes an angle of greater that 45° with $A_1A_2$ and with $A_4A_3$, while a similar statement is true for each generator of the family $\{SS^*\}$.

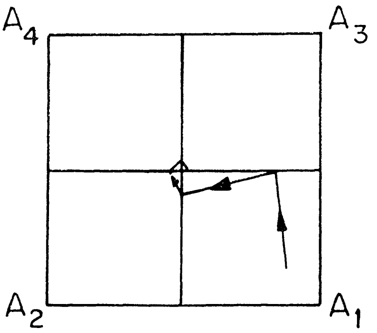


FIG. 4.2. The course of successive iterations as mapped from the surface of constant $\alpha$ ($\alpha = 3$) into the unit square.

Thus, if we denote by $\varphi$ the mapping of the interior of $U$ into itself induced by one complete cycle of the IPFP, the above observation implies that $\varphi$ is a contraction according to the Euclidean metric $\rho$. By this we mean that there exists a constant $\beta$, with $0 < \beta < 1$, such that

$$\rho(\varphi x, \varphi y) \leqq \beta\rho(x, y) \tag{4.2}$$

for any two points, $x$ and $y$, in the interior of $U$. In this case, $\beta^{-1}$ is the slope of the generator of the family $\{TT^*\}$ which passes through the center of $U$. Since $\varphi$ is a contraction mapping, it has one and only one fixed point, the center of the square (Kolmogorov and Fomin, 1957, page 43). Moreover, successive applications of $\varphi$ produce a sequence of points which converge to the fixed point, and the IPFP converges to that table corresponding to the unique fixed point.

The contraction condition (4.2) implies that the convergence is geometric in the sense that, if $p$ is the fixed point and $p^{(N)}$ the point corresponding to that table produced at the $N$th step in the iteration,

$$\rho(p^{(2m)}, p) = \rho(\varphi^m p^{(0)}, \varphi^m p) \leqq \beta^m \rho(p^{(0)}, p), \quad \text{and} \tag{4.3}$$

$$\rho(p^{(2m+1)}, p) = \rho(\varphi^m p^{(1)}, \varphi^m p) \leqq \beta^m \rho(p^{(1)}, p). \tag{4.4}$$

**5. Convergence of IPFP for $r \times c$ tables.** Suppose we consider a simplex $OD_1 \cdots D_{r-1} B_1 \cdots B_{c-1}$ in $(r+c-2)$-space. Then a new polytope is generated by moving the simplex of $r-1$ dimensions, $R \equiv (OD_1 \cdots D_{r-1})$, parallel to itself so that $O$ moves over the whole boundary of the simplex $C \equiv (OB_1 \cdots B_{c-1})$, and the same polytope is generated by interchanging the roles of the two simplices. This polytope is called a *simplotope of type* $(r-1, c-1)$. When $R$ is orthogonal to $C$, the polytope is an *ortho-simplotope of type* $(r-1, c-1)$. We can think of the ortho-simplotope of type $(r-1, c-1)$ as the rectangular product of the simplices $R$ and $C$ (cf. Sommerville, 1958, page 113, and Coxeter, 1963, page 124).

For the $r \times c$ contingency table, Fienberg (1968) indicated that the manifold of constant interaction has co-dimension $(r-1)(c-1)$ with respect to $(rc-1)$-space. The boundary of the intersection of the manifold with the $(rc-1)$-dimensional simplex of reference consists $r$ non-intersecting $(c-1)$-dimensional simplices and $c$ non-intersecting $(r-1)$-dimensional simplices, where each $(c-1)$-simplex meets each $(r-1)$-simplex in exactly one vertex and vice versa. Thus the intersection of the manifold with the $(rc-1)$-simplex of reference is homeomorphic to an ortho-simplotope of type $(r-1, c-1)$. For $r=c=2$, we saw in Section 4 that the ortho-simplotope could be taken as the unit square. For $r=2$ and $c=3$, it becomes a triangular prism.

Now, we map the intersection, $1-1$, onto an ortho-simplotope of type $(r-1, c-1)$ so that (i) boundaries are mapped onto boundaries, (ii) the relative distances between points on each of the $r$ $(c-1)$-simplicial boundaries and between points on each of the $c$ $(r-1)$-simplicial boundaries are preserved, and (iii) incidences between the generators of the manifold are preserved.

Again, without loss of generality we may assume that

$$P_{i\cdot} = 1/r \quad \text{and} \quad p_{\cdot j} = 1/c \qquad \forall\, i, j \tag{5.1}$$

for otherwise the mapping can be redefined to make distances between points on the boundary correspond to the situation where (5.1) is true.

We can now make several observations:

(a) the point corresponding to the table to which we wish to converge is the center of the ortho-simplotope;

(b) the intersection of the $(rc-1)$-dimensional simplex of reference with the $(r-1)$-flats which generate the *manifold of constant interaction* are $(r-1)$-simplices, and similarly the intersection with the generating $(c-1)$-flats are $(c-1)$-simplices;

(c) the $(r-1)$-simplices in (b) are mapped into a family of $(r-1)$-simplices in the ortho-simplotope, each of which intersects all of the $(c-1)$-simplices on the boundary in exactly one point such that the $\mu = \min(r-1, c-1)$ mutually invariant angles (see Sommerville, 1958, page 45) between each $(r-1)$-simplex and each $(c-1)$-simplex are all greater than 45°;

(d) a statement similar to (c) holds true for the $(c-1)$-simplices of (b).

Now, if we denote by $\varphi^*$ the mapping of the interior of the ortho-simplotope into itself, which is induced by one cycle of the IPFP, the above observations imply that $\varphi^*$ is a contraction according to the Euclidean metric $\rho^*$ defined on the ortho-simplotope, i.e., for any two points in the interior, there exists a constant $\beta^*$, with $0 < \beta^* < 1$, such that

$$\rho^*(\varphi^* x, \varphi^* y) \leqq \beta^* \rho^*(x, y). \tag{5.2}$$

We can determine a value for $\beta^*$ as follows. Look at the $(r-1)$-simplex from (c) which passes through the center of the ortho-simplotope and denote by $\theta_1$ the minimum mutually invariant angle which this simplex makes with the $(c-1)$-simplicial boundaries. Similarly denote by $\theta_2$ the corresponding minimum angle between the $(c-1)$-simplex of (d) through the center and the $(r-1)$-simplicial boundaries.

We can then take as our contraction constant

$$\beta^* = \{\tan[\min(\theta_1, \theta_2)]\}^{-1}. \tag{5.3}$$

The contraction condition given by (5.2) and (5.3) implies that the convergence of the IPFP is geometric in the sense of (4.3) and (4.4).

**6. Extensions and discussion.** Deming (1943), Darroch (1962), Caussinus (1965), Bishop (1967, 1969), Mosteller (1968), and Ireland and Kullback (1968) have discussed the generalization of the iterative proportional fitting procedure to multi-dimensional contingency tables. The geometric proofs of Sections 4 and 5 can easily be extended to cover the convergence of these generalizations.

A more involved problem is the extension of the IPFP to situations where the initial values $n_{ij}$ are not all positive, i.e., some $n_{ij}$ are zero. Ireland and Kullback (1968) avoided this extension to simplify their argument. Brualdi, Parter and Schneider (1966) showed that if $r = c$, and if the marginal totals are all equal, then there exists a unique table with these marginal totals and the same cross product ratios as the given table iff the original table, after permutation of rows and columns, can be written as the direct sum of fully indecomposable matrices. This condition clearly does not apply when the margins are unequal. In addition, Bishop and Fienberg (1969) and Goodman (1968) have presented conditions for the convergence of the IPFP, in tables with zero cells, where the margins of the original table are preserved and the interaction structure amongst the non-zero cells is changed to correspond to the hypothesis of "quasi-independence". Fienberg (1970) has shown how the solution of the IPFP in this context corresponds to *unique* maximum likelihood estimates under several related sampling schemes.

The extension of the geometric arguments to problems involving tables with zero entries is quite complex, since such tables correspond to points on the boundaries of the $(rc-1)$-dimensional simplex of reference. The geometrical models require further developments in order to handle the asymmetries introduced by these problems.

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