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Termination of the iterative proportional fitting procedure

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Abstract The iterative proportional fitting procedure (IPF procedure) alternately fits a given nonnegative matrix to given positive row marginals and given positive column marginals. This paper proves that if the IPF procedure terminates, then this has to be within the first two steps.

Keywords Iterative proportional fitting · IPF procedure · Termination

Mathematics Subject Classification (2000) 68W40 · 62H17

1 Introduction

The IPF procedure aims to solve the following problem: Given a nonnegative $k \times \ell$ matrix A and positive marginals, find a nonnegative $k \times \ell$ matrix B which fulfills the given marginals and is biproportional to A. To this end, the IPF procedure generates a sequence of matrices $(A(t))$, called the IPF sequence, by alternately fitting rows and columns to match their respective marginals. The procedure is in use in many disciplines for problems such as calculating maximum likelihood estimators in graphical log-affine models (Lauritzen, 1996, Chapter 4.3.1), ranking webpages (Knight, 2008), determining passenger flows (McCord et al., 2010) or calculating seats in parliaments (Pukelsheim, 2014b, Chapter 14).

We say that the IPF procedure terminates in step T, when T is the smallest number such that the even-step IPF subsequence and the odd-step IPF subsequence replicate themselves after step T. That is, the two subsequences have converged in step T, respectively in step $T + 1$. This paper shows that T only takes the values 0, 1, or 2.

Section 2 specifies the IPF procedure. The termination in the case of a converging IPF sequence is based on linear algebra and discussed in Section 3. This is the first main result. The second main result about the termination in case of a nonconverging IPF

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sequence relies on more sophisticated results and is presented in Section 4. Moreover, a characterization for the termination within two steps is given. Section 5 proposes perspectives for a further generalization.

In the sequel, all indices i belong to the set $\{1, \ldots, k\}$ whereas all indices j belong to the set $\{1, \ldots, \ell\}$. A subscript plus-sign indicates the summation over the index that would otherwise appear in its place. A set as a subscript denotes the summation over all entries belonging to that set, i. e. $r_I = \sum_{i \in I} r_i$. The transposed vector or transposed matrix is indicated by a prime. For all $n \in \mathbb{N}$, we define $\mathbb{1}_n := (1, \ldots, 1)' \in \mathbb{R}^n$.

2 IPF procedure

We specify the IPF procedure in full detail. The *IPF procedure* takes as input a nonnegative matrix $A \in \mathbb{R}^{k \times \ell}_{\geq 0}$ with positive row sums, $a_{i+} > 0$ for all i, and positive column sums, $a_{+j} > 0$ for all j, and two positive vectors $r \in \mathbb{R}^k_{>0}$ and $c \in \mathbb{R}^\ell_{>0}$. The matrix A is referred to as the *input matrix*, whereas the vector r is called the *row marginals* and the vector c is called the *column marginals*. The triple (A, c, r) forms the *input problem*.

The procedure is initialized by setting $A(0) := A$. Subsequently, the *IPF sequence* $(A(t))$ is calculated by iteratively repeating the following two steps:

- Odd steps $t + 1$ fit row sums to row marginals. To this end, all entries in the same row are multiplied by the same multiplier according to

$$a_{ij}(t+1) := \frac{r_i}{a_{i+}(t)} \cdot a_{ij}(t) \text{ for all entries } (i, j). \tag{2.1}$$

- Even steps $t + 2$ fit column sums to column marginals. To this end, all entries in the same column are multiplied by the same multiplier according to

$$a_{ij}(t+2) := \frac{c_j}{a_{+j}(t+1)} \cdot a_{ij}(t+1) \text{ for all entries } (i, j). \tag{2.2}$$

For all steps $t \geq 0$ the inequality $a_{ij}(t) > 0$ holds if and only if $a_{ij} > 0$ holds. Consequently, all row sums $a_{i+}(t)$ and all column sums $a_{+j}(t)$ always stay positive. Thus, the IPF procedure is well defined. We say that the *IPF procedure converges* when the IPF sequence $(A(t))$ converges.

If $A(T) = A(T+2)$ holds for some $T \in \mathbb{N}$, then $A(T+1) = A(T+3)$ holds as well. In this case, the even-step subsequence $(A(t))$ and the odd-step subsequence $(A(t+1))$ stays constant for all even steps $t \geq T$. Therefore, the procedure can be terminated. We say that the IPF procedure *terminates* in step $T \in \mathbb{N}$ when T is the smallest natural number such that $A(T) = A(T+2)$ holds.

As already mentioned by Rüschendorf (1995, p. 1164) and Vejnarová (2003, p. 585), the IPF procedure terminates after at most two steps if the input matrix A is of product form.

Example 2.1 (Input matrix of product form). Let (A, c, r) be an input problem such that for all entries (i, j) and some $u \in \mathbb{R}^k_{>0}, v \in \mathbb{R}^\ell_{>0}$ it holds $a_{ij} = u_i v_j$.

Then, the first three steps of the IPF procedure yield for all entries (i, j) the equations

$$a_{ij}(1) = \frac{r_i}{a_{i+}} a_{ij} = \frac{r_i}{\sum_q u_i v_q} u_i v_j = \frac{r_i}{v_+} v_j, \tag{2.3}$$

$$a_{ij}(2) = \frac{c_j}{a_{+j}(1)} a_{ij}(1) = \frac{c_j}{\sum_p \frac{r_p}{v_+} v_j} \frac{r_i}{v_+} v_j = \frac{r_i c_j}{r_+}, \tag{2.4}$$

$$a_{ij}(3) = \frac{r_i}{a_{i+}(2)} a_{ij}(2) = \frac{r_i}{\sum_q \frac{r_i c_q}{r_+}} \frac{r_i c_j}{r_+} = \frac{r_i c_j}{c_+}. \tag{2.5}$$

Further steps reproduce the matrices $A(2)$ and $A(3)$. Therefore, the IPF procedure terminates in step $T = 2$ at the latest. Moreover, if $c_+ = r_+$ holds, the IPF procedure converges within two steps. ♢

3 Termination in case of convergent IPF procedure

In this section, we discuss the termination in case the IPF procedure is convergent. Then, the condition $A(T) = A(T + 2)$ is equivalent to $A(T) = A(T + 1)$. We show that T only attains the values 0, 1, or 2. To this end, we define $x^2 := (x_1^2, \ldots, x_n^2)$ for all $x \in \mathbb{R}^n$.The following lemma is crucial.

Lemma 3.1 (Quadratic system of equations)**.** *Let $z \in \mathbb{R}^n_{>0}$ be given. Then $x \in \mathbb{R}^n$ is a solution of the system of equations*

$$z'x = z_+, \tag{3.1}$$

$$z'x^2 = z_+, \tag{3.2}$$

if and only if $x = \mathbb{1}_n$.

Proof. Let $x \in \mathbb{R}^n$ be a solution of equation (3.1). It holds

$$z'x^2 = \sum_i z_i x_i^2 = \sum_i z_i(2x_i - 1 + (x_i - 1)^2) = 2\sum_i z_i x_i - \sum_i z_i + \sum_i z_i(x_i - 1)^2 \tag{3.3}$$

$$= 2z'x - z_+ + \sum_i z_i(x_i - 1)^2 = z_+ + \sum_i z_i(x_i - 1)^2 \geq z_+. \tag{3.4}$$

If $x \neq \mathbb{1}_n$ holds, the above inequality is strict. However, this contradicts equation (3.2). Thus, $x = \mathbb{1}_n$ follows. □

Now we are ready to present the first main theorem.

Theorem 3.2 (Termination in the case of a convergent IPF procedure)**.** *If the IPF procedure converges and terminates in step T, then it holds $T \in \{0, 1, 2\}$.*

Proof. The proof is by contradiction.

I. Assume the IPF procedures terminates in an even step $T > 2$, that is $a_{i+}(T) = r_i = a_{i+}(T-1)$ for all i and $a_{+j}(T) = c_j \neq a_{+j}(T-1)$ for some j. To simplify the notation, we define two scaling factors by

$$x := \left(\frac{a_{+1}(T-1)}{c_1}, \dots, \frac{a_{+\ell}(T-1)}{c_\ell}\right)' \quad \text{and} \quad y := \left(\frac{a_{1+}(T-2)}{r_1}, \dots, \frac{a_{k+}(T-2)}{r_k}\right)'. \tag{3.5}$$

II. According to equation (2.2), $A(T-1)$ is a reversed column fit of $A(T)$ and fulfills the row marginals,

$$A(T-1) = A(T)\,\mathrm{Diag}(x), \tag{3.6}$$

$$A(T-1)\mathbb{1}_\ell = A(T)x = r. \tag{3.7}$$

By equation (2.1), $A(T-2)$ is a reversed row fit of $A(T-1)$,

$$A(T-2) = \mathrm{Diag}(y)A(T-1), \tag{3.8}$$

and since we assumed $T > 2$ the matrix $A(T-2)$ fulfills the column marginals,

$$\mathbb{1}_k' A(T-2) = y'A(T-1) = c'. \tag{3.9}$$

III. Substituting equation (3.6) in equation (3.9) we obtain

$$y'A(T)\,\mathrm{Diag}(x) = c'. \tag{3.10}$$

Therefore, it holds

$$y'A(T)x = y'A(T)\,\mathrm{Diag}(x)\mathbb{1}_\ell = c'\mathbb{1}_\ell = c_+ = a_{++}(T). \tag{3.11}$$

IV. Equation (3.7) in combination with $A(T)\mathbb{1}_\ell = r$ yields

$$A(T)x = r = A(T)\mathbb{1}_\ell. \tag{3.12}$$

Applying equation (3.10), $\mathbb{1}_k' A(T) = c'$ and equation (3.12), it holds

$$y'A(T)\,\mathrm{Diag}(x)x = c'x = \mathbb{1}_k' A(T)x = \mathbb{1}_k' A(T)\mathbb{1}_\ell = a_{++}(T). \tag{3.13}$$

Using the notation $x^2 := (x_1^2, \dots, x_\ell^2)$, we rewrite the above equation (3.13) as

$$y'A(T)x^2 = a_{++}(T). \tag{3.14}$$

V. From equation (3.12) and equation (3.11) we derive

$$y'A(T)\mathbb{1}_\ell = y'A(T)x = a_{++}(T). \tag{3.15}$$

Hence, for $z' := y'A(T)$ we have $z_+ = a_{++}(T)$. By definition of the IPF procedure it holds $a_{i+} > 0$ for all i and $a_{+j} > 0$ for all j and therefore it follows $y > 0$ and thus $z > 0$ as well. According to equations (3.11) and (3.14), the vector x has to fulfill the system of equations

$$z'x = z_+, \tag{3.16}$$
$$z'x^2 = z_+ \tag{3.17}$$

with $z > 0$. By Lemma 3.1 the only solution to this system of equations is $x = \mathbb{1}_\ell$. But then $A(T) = A(T-1)$ holds contradicting the assumption $a_{+j}(T-1) \neq c_j$ for some j. Consequently, we conclude $T \in \{0, 1, 2\}$.

VI. The case that the IPF procedure terminates in an odd step $T + 1 > 2$ follows analogously. □

Theorem 3.2 shows that in case of a convergent IPF procedure, the IPF procedure terminates either within the first two steps, or else the convergence happens in the limit. For a termination after two steps the input matrix does not necessarily have to be of product form as shown by the following example.

Example 3.3 (Termination after two steps without product form of input matrix)*.* Let the input problem (A, c, r) be given by

$$A = \begin{pmatrix} 12 & 0 & 4 \\ 6 & 1 & 1 \\ 6 & 2 & 0 \end{pmatrix}, \quad c = (20, 12, 8) \quad \text{and} \quad r = (8, 16, 16). \tag{3.18}$$

Since A contains zero entries, it can not be of a product form. It holds

$$A(1) = \left(\frac{r_i}{a_{i+}} a_{ij}\right)_{ij} = \mathrm{Diag}(1/2, 2, 2)A = \begin{pmatrix} 6 & 0 & 2 \\ 12 & 2 & 2 \\ 12 & 4 & 0 \end{pmatrix} \tag{3.19}$$

and

$$A(2) = \left(\frac{c_j}{a(1)_{+j}} a_{ij}(1)\right)_{ij} = A(1)\,\mathrm{Diag}(2/3, 2, 2) = \begin{pmatrix} 4 & 0 & 4 \\ 8 & 4 & 4 \\ 8 & 8 & 0 \end{pmatrix}. \tag{3.20}$$

Hence, the matrix $A(2)$ fulfills the row marginals as well as the column marginals. Thus, the IPF procedure terminates in the second step. However, starting the IPF procedure with a column fitting step does not result in a termination in the second step. In that case, the IPF procedure terminates in the limit with the same limit matrix $A(2)$. ♢

4 Termination of the IPF sequence

In this section, we examine the termination of the IPF procedure without any further restrictions on the input problem (A, c, r). Thus, the IPF procedure might not converge. In this case, the IPF has at most two accumulation points.

Theorem 4.1 (Accumulation points of the IPF sequence)**.** *Let (A, c, r) be an input problem and $(A(t))$ be the respective IPF sequence. Then the following two statements hold:*

(i) The even-step IPF subsequence $(A(t))_{t=0,2,4,\dots}$ converges.

(ii) The odd-step IPF subsequence $(A(t+1))_{t=0,2,4,\dots}$ converges.

Proof. See Gietl and Reffel (2013, Theorem 5.3). □

To characterize the convergence of the IPF procedure the set of all columns connected in A, $J_A(I) := \{j \in \{1, \dots, \ell\} \mid \exists i \in I : a_{ij} > 0\}$, plays an important role. The input problem (A, c, r) can then be checked for convergence by the flow inequalities according to the following theorem.

Theorem 4.2 (Convergence of the IPF procedure)**.** *Let (A, c, r) be an input problem. Then the IPF procedure converges if and only if $c_+ = r_+$ holds and all row subsets $I \subseteq \{1, \dots, k\}$ fulfill the flow inequalities*

$$r_I \leq c_{J_A(I)}. \tag{4.1}$$

Proof. See Hershkowitz et al. (1997, Theorem 3.2) or Pukelsheim (2014a, Theorem 3). □

We call a nonnegative matrix C *connected* when it is not disconnected. A nonnegative matrix D is *disconnected* when there exists a permutation of rows and a permutation of columns such that D acquires block format,

$$D = \begin{array}{c c} & \begin{array}{cc} J & \overline{J} \end{array} \\ \begin{array}{c} I \\ \overline{I} \end{array} & \begin{pmatrix} D^{(1)} & 0 \\ 0 & D^{(2)} \end{pmatrix} \end{array}, \tag{4.2}$$

where at least one of the subsets $I \subseteq \{1, \dots, k\}$ or $J \subseteq \{1, \dots, \ell\}$ is nonempty and proper. Here, the overline indicates the complement of a set.

The odd-step limit matrix $R^* := \lim_{t=0,2,4,\dots} A(t+1)$ is not necessarily connected. It decomposes into $p \geq 1$ connected submatrices with index sets $I_1 \times J_1, \dots, I_p \times J_p$. For each of these submatrices, a quotient r_{I_n}/c_{J_n}, $n = 1, \dots, p$, can be calculated. We subsume the submatrices with the largest quotients and call this submatrix the *largest block*. Hence, the largest block is a union of several connected submatrices of the matrix R^*. The row set of the largest block is determined by the input problem as follows.

Theorem 4.3 (Row set of the largest Block)**.** *Let A be connected and (A, c, r) be an input problem. Then the set of rows with maximal cardinality among the sets I that maximize the quotient $r_I/c_{J_A(I)}$ is unique and equals the set of rows of the largest block.*

Proof. See Aas (2014, Lemma 3 and Theorem 3) or Reffel (2014, Theorem 10.22). □

The combination of Theorem 4.2 and Theorem 4.3 yield the second main theorem of this paper, a generalization of Theorem 3.2.

Theorem 4.4 (Termination). *If the IPF procedure terminates in step T, then it holds $T \in \{0, 1, 2\}$.*

Proof. I. Without loss of generality we may assume that A is connected. Otherwise the IPF procedure can be applied separately on each input problem consisting of a connected submatrix of A and the respective marginals. Then, the IPF procedure terminates, if every IPF procedure applied on the single input problems terminates.

II. If $c_+ \neq r_+$ holds, we rescale the row marginals to $\tilde{r}_i = (c_+/r_+)r_i$ for all i. As a result, we have $\tilde{r}_+ = c_+$. Let $(\widetilde{A}(t))$ be the IPF sequence obtained from the input problem $(A, c, \tilde{r})$. By an easy induction it holds $\widetilde{A}(t) = A(t)$ and $\widetilde{A}(t+1) = (c_+/r_+)A(t+1)$ for all even steps t. Consequently, we have

$$\min\{T \in \mathbb{N} \mid A(T) = A(T+2)\} = \min\{T \in \mathbb{N} \mid \widetilde{A}(T) = \widetilde{A}(T+2)\}. \tag{4.3}$$

Therefore, we assume without loss of generality $c_+ = r_+$.

III. If the IPF sequence converges, the statement follows from Theorem 4.4. Otherwise, with the assumption made above and by Theorem 4.2, it holds $r_I > c_{J_A(I)}$ for some proper and nonempty subset $I \subset \{1, \dots, k\}$. Hence, the set of rows $\widetilde{I}$ with maximal cardinality among the sets I that maximize the quotient $r_I/c_{J_A(I)}$ has to be a nonempty and proper subset of $\{1, \dots, k\}$ as well. According to Theorem 4.3, the set of rows of the largest block is a proper subset of $\{1, \dots, k\}$. As a result, the odd-step limit matrix R^* is disconnected. Since A is assumed to be connected, some positive entries of A have to converge to 0. But this is only possible in the limit, because all matrices $A(t)$, $t \geq 0$, share the same zero entries. $\square$

From step III of the proof above, the following corollary is immediately.

Corollary 4.5. *Let (A, c, r) an input problem with A connected and $c_+ = r_+$ such that the IPF procedure does not converge. Then the IPF procedure does not terminate and the accumulation points of the IPF sequence are disconnected.*

Input problems such that the IPF procedure terminates after two steps may be characterized in the following way. The asymmetry is caused by fixing the first step of the IPF procedure to be a row fitting (cf. Example 3.3).

Theorem 4.6 (Characterization of input problems). *Let $B \in \mathbb{R}^{k \times \ell}_{\geq 0}$ be connected and define $r := B\mathbb{1}_\ell$ as well as $c := \mathbb{1}_k' B$. Then the input problems (A, r, c) such that the respective IPF procedure converge to the limit matrix B and terminates after at most two steps are of the form*

$$A := \operatorname{Diag}(x) B \operatorname{Diag}(y) \tag{4.4}$$

for an arbitrary $x \in \mathbb{R}^k_{>0}$ and some $y \in (\mathbb{1}_\ell + \ker(B)) \cap \mathbb{R}^\ell_{>0}$.

Proof. I. We show that equation (4.4) is sufficient. Since $By = B\mathbb{1}_\ell = r$, it holds

$$a_{ij}(1) = \frac{r_i}{a_{i+}} a_{ij} = \frac{r_i}{\sum_j x_i b_{ij} y_j} x_i b_{ij} y_j = \frac{r_i}{\sum_j b_{ij} y_j} b_{ij} y_j = \frac{r_i}{r_i} b_{ij} y_j = b_{ij} y_j \quad \text{for all } (i, j). \tag{4.5}$$

From $c = \mathbb{1}_k' B$ we conclude

$$a_{ij}(2) = \frac{c_j}{\sum_i b_{ij} y_j} b_{ij} y_j = \frac{c_j}{\sum_i b_{ij}} b_{ij} = \frac{c_j}{c_j} b_{ij} = b_{ij} \quad \text{for all } (i,j). \tag{4.6}$$

II. To prove the necessity of equation (4.4), observe that by Corollary 4.5 the IPF procedure has to be convergent in order to terminate. Consequently, for some $y \in \mathbb{R}^\ell_{>0}$ it has to hold

$$A(1) = B\,\mathrm{Diag}(y), \quad A(1)\mathbb{1}_\ell = r \quad \text{and} \quad a_{ij}(1)\frac{c_j}{a_{+j}(1)} = b_{ij} \quad \text{for all } (i,j). \tag{4.7}$$

The latter equation is always fulfilled since

$$a_{ij}(1)\frac{c_j}{a_{+j}(1)} = b_{ij} y_j \frac{c_j}{\sum_i b_{ij} y_j} = b_{ij} \frac{c_j}{\sum_i b_{ij}} = b_{ij} \quad \text{for all } (i,j). \tag{4.8}$$

From equations (4.7) it follows $By = r$. Because of $B\mathbb{1}_\ell = r$, we conclude $y \in (\mathbb{1}_\ell + \ker(B)) \cap \mathbb{R}^\ell_{>0}$.

For the input matrix A, it has to hold

$$A = \mathrm{Diag}(x)A(1) \quad \text{and} \quad a_{ij}\frac{r_i}{a_{i+}} = a_{ij}(1) \quad \text{for all } (i,j). \tag{4.9}$$

However, the latter equation holds for all $x \in \mathbb{R}^k_{>0}$ since

$$a_{ij}\frac{r_i}{a_{i+}} = x_i a_{ij}(1)\frac{r_i}{\sum_j x_i a_{ij}(1)} = a_{ij}(1)\frac{r_i}{a_{i+}(1)} = a_{ij}(1) \quad \text{for all } (i,j). \tag{4.10}$$

From equations (4.7) and (4.9) it follows $A = \mathrm{Diag}(x)B\,\mathrm{Diag}(y)$ for an arbitrary $x \in \mathbb{R}^k_{>0}$ and some $y \in (\mathbb{1}_\ell + \ker(B)) \cap \mathbb{R}^\ell_{>0}$. □

5 Outlook

We showed that the IPF procedure may only terminate within the first two steps. If it does not do so, the transition to the limit of the IPF sequence is necessary. This motivates the analysis of the limit behavior of the IPF sequence, which has been examined by Gietl and Reffel (2013) and the literature quoted therein.

A possible generalization of the IPF procedure is the passage from the finite sample space $\{1,\ldots,k\} \times \{1,\ldots,\ell\}$ with the power set as the σ-algebra to an arbitrary sample space $\Omega_1 \times \Omega_2$ with a product σ-algebra $\mathcal{A}_1 \otimes \mathcal{A}_2$. The input matrix is replaced by a bivariate probability distribution and the marginals by univariate probability distributions on the respective measurable spaces. This has been analyzed by Rüschendorf (1995). Theorem 3.2 can be generalized to this setting as well. For details see Reffel (2014, Theorem 3.3). A generalization of Theorem 4.4 seems out of reach at the moment, because only necessary conditions for the convergence of the IPF procedure are available.

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