ON THE MINRES METHOD OF FACTOR ANALYSIS*

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Abstract

The minres method is an effective means for estimating factor loadings under the condition that the sum of squares of the off-diagonal residuals be minimized. This paper is addressed to the efficient implementation and the convergence properties of the method.

Key words: minres method, factor analysis, communality.

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1. Introduction

A basic problem in factor analysis (Harman [4, chap. 5]) is the resolution of n observed variables z_j linearly in terms of a smaller number m of common factors f_p. We assume the classical model:

$$(1.1)\quad z_j = \sum_{p=1}^{m} a_{jp} f_p + d_j u_j \quad \text{for } j = 1,2,\ldots,n ,$$

where a_{jp} are unknown parameters called common-factor loadings, u_j represent the errors or unique factors and d_j are their coefficients, or, in matrix form,

$$(1.2)\quad \mathbf{z} = A\mathbf{f} + D\,\mathbf{u}$$

and A is to be estimated. Once a solution has been found, the fundamental theorem of factor analysis (Thurstone [7, p. 70]) states that a matrix $\hat{R}$ of reproduced correlations is given by

$$(1.3)\quad \hat{R} = AA^T,$$

under the assumption of uncorrelated factors. The diagonal elements of $\hat{R}$ are known as communalities. Our problem is to get a best fit to the observed correlation matrix R° by the reproduced matrix $\hat{R}$.

A least squares fit of the total matrix R° leads to the principal-components method (Harman [4, chap. 8]) and $\hat{R}$ will consist of the m greatest eigenvalues of R° and their corresponding eigenvectors. This method optimally reproduces the total variance of the variables. However, a major objective of factor analysis is to best reproduce the observed correlations. Thurstone [8, p. 61] states, "The object of a factor problem is to account for the tests, or their intercorrelations, in terms of a small number of derived variables, the smallest possible number that is consistent with acceptable residual errors." In [6] Harman and Jones propose to solve this problem by maximally reproducing the off-diagonal elements of the correlation matrix in the least squares sense, that is, they want to minimize the objective function

$$(1.4) \quad f(A) \equiv \sum_{j=1}^{n} \sum_{\substack{k=1 \\ k \neq j}}^{n} \left(r_{jk} - \sum_{p=1}^{m} a_{jp} a_{kp}\right)^2 .$$

The communalities consistent with this factor matrix are given by

$$(1.5) \quad h_j^2 = \sum_{p=1}^{m} a_{jp}^2 \quad \text{for } j = 1,2,\ldots n.$$

Several optimization procedures were investigated in [6]. The conclusion is that a simple Gauss-Seidel approach appears to be most efficient. Harman and Jones call their technique the minres method, for "minimum residuals." But a solution may be obtained for which some communalities exceed unity, a problem called the "generalized Heyword case" (Harman [4, pp. 116-117]). In order that the factor solution be acceptable, Harman and Fukuda [5] modify the minres method to minimize the objective function (1.4) subject to the constraints

$$(1.6) \quad h_j^2 \leq 1 \quad \text{for } j = 1,2,\ldots,n \ .$$

They remark that their modified method is just as efficient as the original approach.

This paper is addressed to the minres method of Harman and Fukuda [5]. We shall study both the efficient implementation and the convergence properties of their method.

2. Minres Method

Harman and Jones [6] adopt the idea of the block Gauss-Seidel technique for linear equations. Their minres method is an iterative procedure in which changes are made to some variables and the new variables then replace the old ones. In fact, changes are made to a row of the factor matrix A at a time, so that the objective function f(A) in (1.4) is but a quadratic function of the displacements.

More explicitly, let

$$(2.1) \qquad A \equiv \begin{bmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_n^T \end{bmatrix}$$

and suppose that we have replaced the j-th row of A by a new row vector

$$(2.2) \qquad \hat{\mathbf{a}}_j^T \equiv (\hat{a}_{j1}, \hat{a}_{j2}, \ldots, \hat{a}_{jm}).$$

The new reproduced correlation of variable j with any other variable k is

$$(2.3) \qquad \hat{r}_{jk} = \sum_{p=1}^{m} a_{kp}\, \hat{a}_{jp},$$

while the sum of squares of residual correlations of variable j with all other variables becomes

(2.4) $$f_j \equiv \sum_{\substack{k=1 \\ k \neq j}}^{n} (r_{jk} - \sum_{p=1}^{m} a_{kp} \hat{a}_{jp})^2.$$

Harman and Jones want to choose the new row such that f_j is minimized. In other words, they want to solve the problem:

(2.5) $$||\mathbf{b}_j - A_{-j} \hat{\mathbf{a}}_j||_2 = \text{minimum},$$

where

(2.6) $$\mathbf{b}_j \equiv (r_{j1}, \ldots, r_{j,j-1}, r_{j,j+1}, \ldots, r_{jn})^T$$

and

(2.7) $$A_{-j} \equiv \begin{pmatrix} \mathbf{a}_1^T \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_{j-1}^T \\ \mathbf{a}_{j+1}^T \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_n^T \end{pmatrix} .$$

Although stable numerical techniques are available for solving the linear least squares problem (2.5) (cf. Golub [2]), Harman and Jones suggest the normal equations approach. They have implicitly assumed that the matrix A_{-j} is of full rank. We shall make the same assumption throughout this paper.

In order that the final result be a meaningful factor analysis solution, Harman and Fukuda [5] replace the key step (2.5) of the minres method by the constrained least squares problem:

$$(2.5) \quad ||\mathbf{b}_j - A_{-j} \hat{\mathbf{a}}_j||_2 = \text{minimum},$$

subject to

$$(2.8) \quad ||\hat{\mathbf{a}}_j||_2 \le 1.$$

Their procedure is to first solve problem (2.5) to check if the constraint (2.8) is satisfied. If the inequality is violated, then the minimum must be attained at a boundary point of the region defined by (2.8). Harman and Fukuda suggest a fairly sophisticated procedure for solving the problem:

$$(2.5) \quad ||\mathbf{b}_j - A_{-j} \hat{\mathbf{a}}_j||_2 = \text{minimum},$$

with an equality constraint

$$(2.9) \quad ||\hat{\mathbf{a}}_j||_2 = 1.$$

The minres method therefore determines factor loadings that minimize the function f(A) for a specified number m of common factors. The fit to the empirical data naturally improves with increasing value of m. The problem of choosing the proper value for m has been investigated by Harman [4, pp. 183-186]. We shall assume a fixed m for this paper.

3. Implementation

We now consider the efficient solution of the linear least squares problem:

(2.5) $||\mathbf{b}_j - A_{-j}\hat{\mathbf{a}}_j||_2^2$ = minimum

using orthogonal triangularization technique (cf. Golub [2]). Let $j \geq 2$. We can assume without loss of generality that we have computed the factorization

(3.1) $A_{-(j-1)} = QR$,

where Q is an $(n-1) \times m$ matrix consisting of orthonormal columns and R is an upper triangular matrix. The two matrices A_{-j} and $A_{-(j-1)}$ differ only in their (j-1)-th row, that is,

(3.2) $A_{-j} = A_{-(j-1)} + \mathbf{e}_{j-1}\mathbf{u}^T$,

where

(3.3) $\mathbf{u} \equiv \mathbf{a}_{j-1} - \mathbf{a}_j$.

We can use an O(nm) procedure from Daniel et al. [1] to compute a QR factorization of A_{-j} from the given factorization of $A_{-(j-1)}$.

Updating the QR Factorization. Let

$$A = QR \in \mathbf{R}^{(n-1)\times m} \quad (n-1 > m)$$

and

$$\bar{A} = A + \mathbf{v}\mathbf{u}^T.$$

Observe that

$$\bar{A} = (Q,\mathbf{v}) \binom{R}{\mathbf{u}^T}.$$

Step 1. Apply the Gram-Schmidt process (with reorthogonalization) to obtain

$$(Q,\mathbf{v}) = (Q,\mathbf{q})\begin{pmatrix} I & \mathbf{r} \\ o & p \end{pmatrix}, Q^T\mathbf{q} = \mathbf{0}, ||\mathbf{q}||_2 = 1.$$

We then have

$$\bar{A} = (Q,\mathbf{q})[\binom{R}{\mathbf{0}^T} + \binom{\mathbf{r}}{p}\mathbf{u}^T] = \tilde{Q}\tilde{R},$$

and $\tilde{Q}$ has orthonormal columns.

Step 2. Choose Givens matrices $G_{n,n+1}, G_{n-1,n}, \ldots, G_{1,2}$ so that

$$G\binom{\mathbf{r}}{p} \equiv G_{1,2} \cdots G_{n,n+1}\binom{\mathbf{r}}{p} \equiv \tau\mathbf{e}_1.$$

That is, choose the $G_{i,i+1}(i=n,n-1,\ldots,1)$ to successively introduce zeroes into the vector from the bottom element through the second. The matrix G is orthogonal. The $(n+1)\times n$ matrix

$$G\binom{R}{\mathbf{0}^T} \equiv G_{1,2} \cdots G_{n,n+1}\binom{R}{\mathbf{0}^T} \equiv R'$$

is upper Hessenberg, and so is

$$G\tilde{R} = R' + \tau\mathbf{e}_1\mathbf{u}^T \equiv \hat{R}.$$

Moreover, by the orthogonality of G, the matrix $\tilde{Q}G^T = \tilde{Q}G_{n,n+1}\cdots G_{1,2} \equiv \hat{Q}$ has orthonormal columns and $\bar{A} = \hat{Q}\hat{R}$.

Step 3. Choose Givens matrices $H_{1,2}, H_{2,3}, \ldots, H_{n,n+1}$ to successively annihilate the subdiagonal elements of $\hat{R}$, giving

$$H\hat{R} \equiv H_{n,n+1} \cdots H_{1,2}\hat{R} \equiv \binom{\bar{R}}{\mathbf{0}^T}$$

with $\bar{R}$ upper triangular. Then

$$\hat{Q}H^T = \hat{Q}\, H_{1,2} \cdots H_{n,n+1} \equiv (\bar{Q}, \bar{\mathbf{q}})$$

has orthonormal columns and

$$\bar{A} = (\bar{Q}, \bar{\mathbf{q}})\begin{pmatrix} \bar{R} \\ \mathbf{0}^T \end{pmatrix} = \bar{Q}\,\bar{R},$$

as required. □

This procedure uses approximately $2(k+3)nm + 3m^2$ multiplications and additions, where k is the number of orthogonalization steps (k-1 reorthogonalization). It is because Daniel et al. have devised a clever scheme implementing a Givens transformation on a 2×m matrix using 3m multiplications and additions, instead of the usual 4m multiplications and 2m additions. There is a further saving of nm multiplications and additions due to the fact that

$$\mathbf{v} = \mathbf{e}_{j-1}\ .$$

The updating algorithm simplifies for the square case when $n-1 = m$. As Q is now orthogonal, we get

$$\bar{A} = Q(R+\mathbf{r}\mathbf{u}^T), \qquad \mathbf{r} \equiv Q^T\mathbf{v}.$$

We then apply Steps 2 and 3, with one fewer Givens transformation each, to compute the desired factorization.

Let us consider the case when j=1. We can assume the factorization

$$A_{-n} = QR.$$

Let P be the permutation matrix of order n-1:

$$P = \begin{bmatrix} \mathbf{e}_{n-1}^T \\ \mathbf{e}_1^T \\ \mathbf{e}_2^T \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{e}_{n-2}^T \end{bmatrix} .$$

Then,

$$PA_{-1} = A_{-n} + \mathbf{e}_1(\mathbf{a}_n^T - \mathbf{a}_1^T).$$

The updating algorithm can now be applied to obtain the factorization:

$$A_{-n} + \mathbf{e}_1(\mathbf{a}_n^T - \mathbf{a}_1^T) = \overline{QR},$$

or

$$A_{-1} = (P^T\overline{Q})\overline{R},$$

as desired.

With the factorization

(3.4) $A_{-j} = \overline{QR},$

the solution to the least squares problem (2.5) is given by

(3.5) $\hat{\mathbf{a}}_j = \overline{R}^{-1}\overline{Q}^T\mathbf{b}_j,$

which requires only $(nm + m^2/2)$ multiplications and additions.

As described in the last section, the minres method now checks the constraint

(2.8) $||\hat{\mathbf{a}}_j|| \leq 1$.

If the inequality is not valid, minres will solve the constrained problem:

(2.5) $||\mathbf{b}_j - A_{-j}\hat{\mathbf{a}}_j||_2$ = minimum,

subject to

(2.9) $||\hat{\mathbf{a}}_j||_2 = 1$.

Golub [3] gives a very efficient algorithm for the linear least squares problem:

(3.6) $||\mathbf{b} - A\mathbf{x}||_2$ = minimum,

with a quadratic constraint

(3.7) $||\mathbf{x}||_2 = 1$.

Define the function

(3.8) $\phi(\mathbf{x},\lambda) = (\mathbf{b}-A\mathbf{x})^T(\mathbf{b}-A\mathbf{x}) + \lambda(\mathbf{x}^T\mathbf{x}-1)$,

where λ is a Lagrange multiplier. Differentiating (3.8) with respect to $\mathbf{x}$ and setting the result to zero, we obtain the equation

(3.9) $(A^TA+\lambda I)\mathbf{x} = A^T\mathbf{b}$.

The parameter λ is positive as our problem assumes that

$$1 < ||A^+\mathbf{b}||_2.$$

We now substitute

$$\mathbf{x} = (A^TA+\lambda I)^{-1}A^T\mathbf{b},$$

into equation (3.7) to obtain

(3.10) $\mathbf{b}^T A(A^T A+\lambda I)^{-2} A^T \mathbf{b}-1 = 0.$

Repeatedly using the identity

$$\det \begin{pmatrix} X & Y \\ Z & W \end{pmatrix} = \det(X)\det(W-ZX^{-1}Y) \quad \text{if } \det(X)\neq 0,$$

we can reduce (3.10) to

(3.11) $\det [(A^T A+\lambda I)^2 - A^T \mathbf{b}\ \mathbf{b}^T A] = 0.$

Finally, let

(3.12) $A = U\Sigma V^T$

be the singular value decomposition of A. Then

(3.13) $A^T A = VDV^T,\ V^T V = I$ and $D = \Sigma^T \Sigma.$

Equation (3.11) becomes

(3.14) $\det [(D+\lambda I)^2 - \mathbf{u}\mathbf{u}^T] = 0$,

where

(3.15) $\mathbf{u} = \Sigma^T U^T \mathbf{b}.$

Golub [3] remarks that the largest real root λ^* of equation (3.14) is the desired value of the Lagrange multiplier and that this root is unique in the open interval $(0, ||\mathbf{u}||_2)$.

Our constrained problem has thus been reduced to that of computing an eigenvalue of the sum of a diagonal matrix and a matrix of rank one. An effective solution technique is again given by Golub in [3]. Suppose that the elements of $\mathbf{u}$ (and hence also of D) have been reordered so that

(3.16) $u_1 = u_2 = \cdots = u_{p-1} = 0$ and $0 < |u_p| \le |u_{p+1}| \le \cdots \le |u_n|$.

Define the bidiagonal matrix

$$(3.17) \qquad K = \begin{bmatrix} 1 & r_1 & & & 0 \\ & 1 & r_2 & & \\ & & \ddots & \ddots & \\ & & & 1 & r_{n-1} \\ 0 & & & & 1 \end{bmatrix}$$

with

$$r_i = \begin{cases} 0 & \text{for } i<p, \\ -u_i/u_{i+1} & \text{for } i \ge p. \end{cases}$$

Note that $|r_i| \le 1$ and

(3.18) $K\mathbf{u} = u_n \mathbf{e}_n$.

Equation (3.14) is equivalent to

(3.19) $\det [G(\lambda)] = 0$,

where

(3.20) $G(\lambda) \equiv K(D+\lambda I)^2 K^T - u_n^2 \mathbf{e}_n \mathbf{e}_n^T$.

The matrix $G(\lambda)$ is tridiagonal so that its determinant is readily computable. As both upper and lower bounds on the root λ^* are known, its value can be determined by applying linear interpolation to equation (3.19). The solution to the constrained problem is now given by

(3.20) $\mathbf{x} = V(D+\lambda^* I)^{-1}\, \mathbf{u}$.

4. Convergence

This section is devoted to the convergence properties of the minres method. We are unaware of any similar results in the literature.

Define a major iteration cycle of the minres method as one consisting of the n constrained problems:

$$(2.5) \quad ||\mathbf{b}_j - A_{-j}\hat{\mathbf{a}}_j||_2 = \text{minimum},$$

subject to

$$(2.8) \quad ||\hat{\mathbf{a}}_j|| \le 1,$$

for j=1,2,...,n. Suppose that an initial matrix A has been chosen to satisfy the inequalities (2.8). Recall the objective function

$$(1.4) \quad f(A) \equiv \sum_{i=1}^{n} \sum_{\substack{k=1 \\ k\neq i}}^{n} (r_{ik} - \sum_{p=1}^{m} a_{ip}a_{kp})^2.$$

For a specified j, we can rewrite the definition as

$$(4.1) \quad f(A) \equiv \sum_{\substack{i=1 \\ i\neq j}}^{n} \sum_{\substack{k=1 \\ k\neq i,j}}^{n} (r_{ik} - \sum_{p=1}^{m} a_{ip}a_{kp})^2$$

$$+ 2 \sum_{\substack{k=1 \\ k\neq j}}^{n} (r_{jk} - \sum_{p=1}^{m} a_{jp}a_{kp})^2.$$

It is obvious that f(A) is nonincreasing as the iteration continues. In particular, let A^c and A^- be the factor matrices at the end of the current and the previous major iteration cycles, respectively. We always have

(4.2) $f(A^c) \le f(A^-)$,

with equality if and only if $A^c = A^-$. We therefore stop iterating when $A^c = A^-$, at which time the jth row of A^c is the solution to the constrained problem:

(2.5) $||\mathbf{b}_j - A_{-j}\hat{\mathbf{a}}_j||_2$ = minimum,

subject to

(2.8) $||\hat{\mathbf{a}}_j||_2 \le 1$,

for $j=1,2,\ldots,n$. Since

$$f(A) \ge \sum_{j=1}^{n} \{ \min_{||\mathbf{a}_j||_2 \le 1} \sum_{\substack{k=1 \\ k \ne j}}^{n} (r_{jk} - \sum_{p=1}^{m} a_{jp}a_{kp})^2 \},$$

we conclude that f(A) achieves its minimum when $A^c = A^-$.

5. Canonical Form

It is well known (cf. Harman [4, pp. 27-28]) that a factor solution for a correlation matrix usually produces a unique factor space but not a unique set of common-factor loadings. For our problem, let us define the reduced correlation matrix as

(5.1) $R^{HSQ} \equiv R^\circ - I + \mathrm{Diag}(AA^T)$.

That is, R^{HSQ} has the computed communalities in the principal diagonal. Our objective function f(A) is now given by

$$\begin{aligned} (5.2) \quad f(A) &= ||R^{HSQ} - AA^T||_F^2 \\ &= ||R^{HSQ} - (AQ)(AQ)^T||_F^2, \end{aligned}$$

where Q is any orthogonal matrix of order m.

Following Harman [4, pp. 164-166] we select a canonical form such that successive factors account for maximum possible variance in the common-factor space determined by the original solution. Consider an n×m factor matrix A, with the singular value decomposition:

$$(5.4)\quad A = U\Sigma V^T,$$

where $U \in \mathbf{R}^{n\times m}$, and $V \in \mathbf{R}^{m\times m}$. Its canonical form is given by the matrix B, where

$$(5.5)\quad B = U\Sigma.$$

The minres method rotates the last determined factor matrix to canonical form after the factor loadings have converged.

6. Test Examples

We have applied the minres method to some well known examples. Our initial factor matrix A consists of the first m principal components of the observed correlation matrix R°. As the diagonal elements of R° all equal unity, it follows that our starting matrix satisfies

$$(2.8)\quad ||a_j||_2 \le 1,$$

for j=1,2,...,n. We stop iterating when

$$(5.1)\quad \max_{j,k} |a^c_{jk} - a^-_{jk}| < 10^{-3},$$

where $A^c \equiv (a^c_{jk})$ and $A^- \equiv (a^-_{jk})$ are the factor matrices at the end of the current and the previous major iteration cycles, respectively.

1. Five Hypothetical Variables [5, p. 569].

This classical example is frequently used to illustrate the Heywood case. The observed correlation marix is given in the upper triangle of Table 1. If the values 1.10, .81, .64, .49, .36 are placed in the diagonal of this matrix, its rank will be one. Hence a single factor with loadings (1.05, .90, .80, .70, .60) will reproduce the correlations with zero residuals. But this factor solution is inadmissible. A proper minres method with one factor is exhibited in Table 1. The total number of iterations is 5 and there are 4 times when the inequality constraint (2.8) is violated. However, since m=1, the least squares problem (2.5) with the equality constraint (2.9) always has the trivial solution ± 1, whose sign will be chosen according to that of the solution to the unconstrained problem (2.5).

Table 1

Variable	Correlations and Residuals*				
j	1	2	3	4	5
1		.945	.840	.735	.630
2	.033		.720	.630	.540
3	.031	-.018		.560	.480
4	.028	-.015	-.012		.420
5	.025	-.012	-.010	-.008	

*Correlations in upper triangle, residuals in lower triangle.

Variable j	a_{j1}	h_j^2
1	1.000	1.000
2	.912	.832
3	.809	.655
4	.707	.500
5	.605	.366
Variance	3.353	3.353

2. Five Socio-Economic Variables [4, p.14].

We present a simple example and an analysis based on two common factors. The details are given in Table 2. The minres method requires 4 iterations and 2 solutions of the least squares problem with a quadratic constraint.

Table 2

Variable	Correlations and Residuals*				
j	1	2	3	4	5
1. Total population		.010	.972	.439	.022
2. Median school years	-.017		.154	.691	.863
3. Total employment	.002	.019		.515	.122
4. Misc. profess. services	.005	-.002	-.005		.778
5. Median value house	.001	-.000	-.013	.002	

*Correlations in upper triangle, residuals in lower triangle.

Variable j	a_{j1}	a_{j2}	h_j^2
1	.621	-.784	1.000
2	.701	.521	.763
3	.701	-.682	.957
4	.881	.144	.797
5	.781	.606	.977
Variance	2.756	1.739	4.495

3. Eight Physical Variables [6, p. 364].

We give the details of a minres solution for m = 2 in Table 3. the total number of iterations is 6 and there is no call to Golub's routine.

Table 3

Variable	Correlations and Residuals*							
j	1	2	3	4	5	6	7	8
1. Height		846	805	859	473	398	301	382
2. Arm span	-014		881	826	376	326	277	415
3. Length of forearm	-020	027		801	380	319	237	345
4. Length of lower leg	037	-020	-011		436	329	327	365
5. Weight	016	-025	007	008		762	730	629
6. Bitrochanteric diameter	018	-006	011	-027	008		583	577
7. Chest girth	-021	004	-014	029	012	-026		539
8. Chest width	-024	044	-002	-020	-027	021	015	

*Correlations in upper triangle, residuals in lower triangle; decimal points omitted.

Variable j	a_{j1}	a_{j2}	h_j^2
1	.856	-.324	.838
2	.848	-.412	.889
3	.808	-.409	.821
4	.831	-.342	.808
5	.750	.571	.889
6	.631	.492	.640
7	.569	.510	.583
8	.607	.351	.492
Variance	4.449	1.510	5.959

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