Multivariate Verfahren 2

factor analysis

Helmut Waldl

May 7th and 8th 2012

factor analysis

principal component analysis

According to the factor analysis model with k factors we try to decompose the data matrix of the standardized data:

$$Z = \underbrace{F}_{(n \times k)} \cdot \underbrace{L^T}_{(k \times p)} + \underbrace{E}_{(n \times p)}$$

We proceed merely descriptive: Z is approximated by a linear combination of k orthonormal vectors of factor values such that E is "minimized"

Contrary to ML factor analysis we do not need a stochastic model with various assumptions for the data, we describe the data directly.

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With principal component analysis we use the first k principal components $F_1, \ldots, F_k$ of the principal axis transformation as factors to describe the standardized data Z, the last $p-k$ principal components are neglected.

We only need a criterion for the determination of the number of factors k.

The complete principal component partition yields

$$Z = F \cdot L^T \qquad F = (F_1 \ldots F_p) \qquad L = (l_1 \ldots l_p) \qquad L = T \cdot \Lambda^{\frac{1}{2}}$$

with $R = L \cdot L^T$.

The part of the complete variance $p = \mathrm{tr}(R)$ of the standardized data explained by the jth factor is

$$\mathrm{tr}((F_j l_j^T)^T (F_j l_j^T)) = \mathrm{tr}(l_j \cdot l_j^T) = \sum_{i=1}^{p} l_{ij}^2 = \lambda_j$$

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If we choose k factors then the principal component analysis estimates the model as follows:

$$Z = F^{(k)} L^{(k)T} + E^{(k)} \qquad \text{with } F^{(k)} = (F_1 \ldots F_k),$$

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further

$$R = L^{(k)} L^{(k)T} + U^{(k)} \qquad \text{with } U^{(k)} = E^{(k)T} E^{(k)}$$

Unlike the fundamental theorem of factor analysis $U^{(k)}$ in general is no diagonal matrix. Therefore from the factor analytical point of view principal component analysis is only an approximative method.

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With k given the principal component analysis yields least square solutions for the k-factor model in the following sense:

$$\mathrm{tr}((Z - F^{(k)} L^{(k)T})^T (Z - F^{(k)} L^{(k)T})) = \mathrm{tr}(R - L^{(k)} L^{(k)T}) =$$

$$= \sum_{i=k+1}^{p} \lambda_i = \min_{\underset{(n\times k)}{F},\underset{(p\times k)}{L}} \{\mathrm{tr}((Z - F \cdot L^T)^T (Z - F \cdot L^T))\}$$

with orthonormal F

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determination of k

1. All principal components F_j with an associated eigenvalue $\lambda_j \geq 1$ included, i.e. all components that explain more than the average variance of one variable ("eigenvalue-criterion"): $k = \max\{j \mid \lambda_j \geq 1\}$
2. We include principal components until a predetermined portion c of the total variance p is reached: $k = \min\{r \mid \lambda_1 + \cdots + \lambda_r \geq c \cdot p\}$
3. With independently normal distributed data the eigenvalues of the empirical covariance matrix have a smooth and uniformly descending graph if we sort and plot them. However with dependent data we mostly find a clear break. Before the break we have relatively big eigenvalues, afterwards the eigenvalues are small and about the same size.

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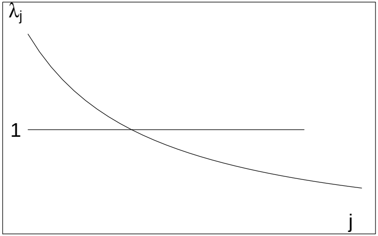
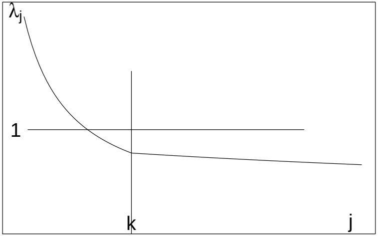


independent variables



dependent variables

We assume the principal components affiliated with eigenvalues after the break as random and choose the position of the break as number of factors k (*Scree-test*, *scree-plot*).

factor analysis

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4. Significance inspection of the principal components according to Bartlett.
   Assumption: normal distribution of the data.

   We test whether the $p - k$ smallest eigenvalues of R differ from each other or not:

   $$H_0(k) : \lambda_{k+1} = \lambda_{k+2} = \cdots = \lambda_p$$

   We start with a small k_0 (stepwise extraction) and include principal components until H_0 is **not** rejected for the first time.

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determination of k

The test statistic

$$U_k = (n-1)\cdot \underbrace{\left(-\ln|R| + \ln(\lambda_1 \cdot \ldots \cdot \lambda_k)\right) + (p-k)\cdot \ln \frac{p-\lambda_1-\cdots-\lambda_k}{p-k}}_{\ln \frac{\prod_{i=1}^{k}\lambda_i \cdot \left(\frac{p-\sum_{i=1}^{k}\lambda_i}{p-k}\right)^{p-k}}{\prod_{i=1}^{p}\lambda_i}}$$

is approximatively $\chi^2_{d_k}$-distributed (caution: not asymptotical) under H_0 with degrees of freedom $d_f = \frac{1}{2}(p-k+2)(p-k-1)$

Remark: under H_0 we have $|R| = \prod_{i=1}^{k}\lambda_i \cdot \left(\frac{p-\sum_{i=1}^{k}\lambda_i}{p-k}\right)^{p-k}$

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principal factor analysis

We start with the factor analysis model and the fundamental theorem $\Sigma = L \cdot L^T + V$

We try to partition the empirical correlation matrix according to the fundamental theorem: $R = L \cdot L^T + V$ with $V = \mathrm{diag}\{v_1^2, \ldots, v_p^2\}$. The communalities $h_i^2 = 1 - v_i^2$ are also combined to a diagonal matrix $K = I - V$

The principal factor analysis is made up of two steps:

1. The specific variances v_i^2 are estimated, in fact via the communalities
2. We perform a principal axis transformation with the reduced empirical correlation matrix $R_h = R - V$:
   $\Lambda = \mathrm{diag}\{\lambda_1, \ldots, \lambda_p\}$ with $\lambda_1 \geq \ldots \geq \lambda_p$ eigenvalues of R_h and $t_1, \ldots, t_p$ the corresponding normalized eigenvectors.

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With $T = (t_1 \cdots t_p)$ and $L = T \cdot \Lambda^{\frac{1}{2}}$ we have

$$L \cdot L^T = T \cdot \Lambda \cdot T^T = R_h$$

We get the factor values with

$$Z = F \cdot \Lambda^{\frac{1}{2}} T^T \qquad \Longleftrightarrow \qquad F = Z \cdot T \cdot \Lambda^{-\frac{1}{2}}$$

and therefore

$$F = Z \cdot \underbrace{T \cdot \Lambda^{-\frac{1}{2}} \overbrace{\Lambda^{-\frac{1}{2}} \overbrace{T^T T}^{I} \cdot \Lambda^{\frac{1}{2}}}^{I}}_{} = Z \cdot \underbrace{T \cdot \Lambda^{-\frac{1}{2}}\Lambda^{-\frac{1}{2}} T^T}_{R_h^{-1}} \underbrace{T \cdot \Lambda^{\frac{1}{2}}}_{L} = Z \cdot R_h^{-1} L$$

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$F = (F_1 \cdots F_p)$. $F_1, \ldots, F_p$ are called **principal factors**, they explain the variances $\lambda_1, \ldots, \lambda_p$. Here we have: $\sum_{i=1}^{p} \lambda_i = \sum_{i=1}^{p} h_i^2$

Caution: here we may have eigenvalues ≤ 0. Such eigenvalues yield meaningless factors. That´s why we limit ourself to the first k principal factors $F_1, \ldots, F_k$ as with principal component analysis.

$$Z = F^{(k)} L^{(k)T} + E^{(k)}$$

$$R = \underbrace{L^{(k)} L^{(k)T} + \overbrace{\sum_{i=k+1}^{p} l_i l_i^T}^{U^{(k)}}}_{R_h} + V$$

As with principal component analysis $U^{(k)}$ in general is not diagonal, i.e. also principal factor analysis is only an approximative method from the factor analysis point of view.

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The two steps of principal factor analysis may be repeated iteratively:

We start e.g. with $V_0 = 0$ or $V_0 = I - K_0$ where in K_0 there are first estimates for the communalities. With this we get:

$$R - V_0 = L_1^{(k)} L_1^{(k)T} + \sum_{i=k+1}^{p} l_{1i} l_{1i}^T$$

$$\text{and } R = L_1^{(k)} L_1^{(k)T} + U_1^{(k)} \text{ respectively}$$

where $U_1^{(k)} = V_0 + \sum_{i=k+1}^{p} l_{1i} l_{1i}^T$

$K_1 = \mathrm{diag}(L_1^{(k)} L_1^{(k)T})$ is the new estimator for the diagonal matrix of communalities, $V_1 = \mathrm{diag}(U_1^{(k)})$ is the new estimator for the specific variances.

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Now we perform a principal axis transformation of $R - V_1 = L_2^{(k)} L_2^{(k)T} + \sum_{i=k+1}^{p} l_{2i} l_{2i}^T$ and $R = L_2^{(k)} L_2^{(k)T} + U_2^{(k)}$ respectively etc.

After an appropriate termination condition is met, e.g. $\frac{\|V_n - V_{n-1}\|}{\|V_n\|} < \varepsilon$ or after a predetermined number of iteration steps, the iterations are stopped.

Then we have $R = L_n^{(k)} L_n^{(k)T} + U_n^{(k)},\ V_n = \text{diag}(U_n^{(k)})$ and the estimated factor values are $F_n^{(k)} = Z \cdot \underbrace{(R - V_n)^{-1}}_{R_h^{-1}} L_n^{(k)}$

Usually the number of factors remains constant during the iterations, however k may be redetermined after each iteration step.

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Now we perform a principal axis transformation of $R - V_1 = L_2^{(k)} L_2^{(k)T} + \sum_{i=k+1}^{p} l_{2i} l_{2i}^T$ and $R = L_2^{(k)} L_2^{(k)T} + U_2^{(k)}$ respectively etc.

After an appropriate termination condition is met, e.g. $\frac{\|V_n - V_{n-1}\|}{\|V_n\|} < \varepsilon$ or after a predetermined number of iteration steps, the iterations are stopped.

Then we have $R = L_n^{(k)} L_n^{(k)T} + U_n^{(k)},\ V_n = \mathrm{diag}(U_n^{(k)})$ and the estimated factor values are $F_n^{(k)} = Z \cdot \underbrace{(R - V_n)^{-1}}_{R_h^{-1}} L_n^{(k)}$

Usually the number of factors remains constant during the iterations, however k may be redetermined after each iteration step.

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Caution:

- The described iteration need not always converge.
- If the iterations converge the limit may be a meaningless solution, i.e. if $K_n \stackrel{n\to\infty}{\longrightarrow} K = \mathrm{diag}\{h_1^2, \ldots, h_p^2\}$ and $V_n \stackrel{n\to\infty}{\longrightarrow} V = \mathrm{diag}\{v_1^2, \ldots, v_p^2\}$ then possibly $h_i^2 > 1$ and $v_i^2 < 0$

If in the iteration process specific variances $v_i^2 < 0$ appear for the first time most statistics software packages stop the iterations with the last appropriate solution (**Heywood-case**).

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estimation of communalities

With the above iterative procedure of the principal factor analysis the communalities are estimated with the model parameters k, L and V.

We may also estimate the communalities independently of k and L, and that with the **multiple correlation coefficient** ρ_j of the standardized data $Z = (z_1, \ldots, z_p)$

$$\rho_j = \frac{\sqrt{\sigma_{(j)} \Sigma_{22}^{-1} \sigma_{(j)}^T}}{\sigma_j} \qquad \text{where}$$

$$Cov(z_j, z_1, \ldots, z_{j-1}, z_{j+1}, \ldots, z_p) = \begin{pmatrix} \sigma_j^2 & \sigma_{(j)} \\ \sigma_{(j)}^T & \Sigma_{22} \end{pmatrix}$$

Consider the order of the variates z!

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ρ_j specifies the maximal correlation between z_j and all possible linear combinations of the remaining z_i $i \neq j$.

$\Longrightarrow$ the variance z_j has in common with the remaining z_i $i \neq j$ is at least ρ_j^2, i.e. $h_j^2 \geq \rho_j^2$

As estimator for ρ_j^2 we use

$$\widehat{\rho_j^2} = r_j^2 = 1 - \frac{1}{r^{jj}}$$

where r^{jj} is the jth diagonal element of R^{-1}. We have

$$r_j^2 \xrightarrow[]{\substack{p \to \infty \\ \frac{k}{p} \to 0}} h_j^2$$

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