Statistics 135

Chapter 9
Factor Analysis

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Purpose of Factor Analysis

Describe the covariance relationship among many variables in terms of a few underlying but unobservable quantities.

Examples:

- Wechsler Adult Intelligence Scale Subtest Scores. The data set consists of 11 variables measuring aspects of intellectual performance; we can think of underlying, unobserved factors that "explain" performance on these tasks; the idea is to identify underlying factors such as verbal ability similar to principal components.
- 2 Fowl bone dimensions where measurements were taken on the skull (2), the wing (2) and the leg (2) for a total of 6 measurements; question: are there underlying commonalities that explain the observed measurements?
- 3 Example 9.3 on page 491: consumer preference data; there are 5 variables: taste, good buy for money, flavor, suitable for snack, provides lots of energy; question: do these variables form groups

The Model

Let $\mathbf{X} \sim N_p(\mu, \mathbf{\Sigma})$ be a p-variate normal vector and $\tilde{\mathbf{X}} = \mathbf{X} - \mu$ is the centered version;

Suppose $F_1, ..., F_m$ are uncorrelated variables m < p with $E[\mathbf{F}] = \mathbf{0}$ and $Cov(\mathbf{F}) = E[\mathbf{FF'}] = \mathbf{I}$.

Consider the model

$$\tilde{X}_{1} = l_{11}F_{1} + l_{12}F_{2} + \dots + l_{1m}F_{m} + \epsilon_{1}$$

$$\tilde{X}_{2} = l_{21}F_{1} + l_{22}F_{2} + \dots + l_{2m}F_{m} + \epsilon_{2}$$

$$\vdots$$

$$\tilde{X}_{p} = l_{p1}F_{1} + l_{p2}F_{2} + \dots + l_{pm}F_{m} + \epsilon_{p}$$

where $E[\epsilon] = \mathbf{0}$ and $Cov(\epsilon) = E[\epsilon \epsilon'] = \mathbf{\Psi} = diag(\psi_1, ... \psi_p)$ and $Cov(\mathbf{F}, \epsilon) = \mathbf{0}_{p \times m}$

Definitions:

- 1 The coefficients l_{ij} for i = 1, ..., p and j = 1, ..., m are called the loadings of the i^{th} variable on the j^{th} factor.
- 2 $F_1, ..., F_m$ are called the common factors.
- 3 $\epsilon_1, ..., \epsilon_p$ are called the errors or specific factors.
- 4 The Orthogonal Factor Model with m Common Factors is given by:

$$\mathbf{X} = \mu + \mathbf{LF} + \epsilon$$

where \mathbf{L} is the matrix of factor loadings and \mathbf{F} is the vector of common factors.

Note:

$$(\mathbf{X} - \mu)(\mathbf{X} - \mu)' = (\mathbf{LF} + \epsilon)(\mathbf{LF} + \epsilon)'$$
$$= \mathbf{LF}(\mathbf{LF})' + \epsilon(\mathbf{LF})' + (\mathbf{LF})\epsilon' + \epsilon\epsilon'$$

and therefore

$$\Sigma = LE[FF'](L)' + E[\epsilon F']L' + LE[F\epsilon'] + \epsilon \epsilon' = LL' + \Psi$$

5 $Cov(\mathbf{X} - \mu) = Cov(\mathbf{X}) = \mathbf{L}\mathbf{L}' + \mathbf{\Psi}$ which gives

$$Var(X_i) = l_{i1}^2 + l_{i2}^2 + ... + l_{im}^2 + \psi_i$$

$$Cov(X_i, X_k) = l_{i1}l_{k1} + l_{i2}l_{k2} + ... + l_{im}l_{km}$$

therefore

$$Cov(X_i, F_j) = l_{ij}$$

6 The variance of X_i is the sum of the specific variance ψ_i and the communality

$$h_i = l_{i1}^2 + l_{i2}^2 + \dots + l_{im}^2$$

7 Most covariance matrices cannot be factored as $\mathbf{L}\mathbf{L}' + \mathbf{\Psi}$ with m << p; for an illustration see example (9.2) on page 486. The solution that is obtained leads to values for correlations that are greater than 1.

8 Factor loadings \mathbf{L} are not unique and can be determined only up to an orthogonal matrix \mathbf{T} . Recall, for orthogonal matrices \mathbf{T} we have $\mathbf{T}\mathbf{T}' = \mathbf{T}'\mathbf{T} = \mathbf{I}$; therefore

$$\mathbf{X} - \mu = \mathbf{LF} + \epsilon = \mathbf{LTT'F} + \epsilon$$

for $L^* = LT$ and $F^* = T'F$ and

$$E(\mathbf{F})^* = \mathbf{T}'E(\mathbf{F}) = \mathbf{0}$$

$$Cov(\mathbf{F}^*) = \mathbf{T}'Cov(\mathbf{F})\mathbf{T} = \mathbf{T}'\mathbf{T} = \mathbf{I}$$

and therefore

$$oldsymbol{\Sigma} = \mathbf{L}\mathbf{L}' + oldsymbol{\Psi} = \mathbf{L}\mathbf{T}\mathbf{T}'\mathbf{L}' + oldsymbol{\Psi} = (\mathbf{L}^*)(\mathbf{L}^*)' + oldsymbol{\Psi}$$

Samples and Estimation

- 1 Sample $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n$ of p-variate observations; it is assumed that the components of \mathbf{X} are correlated, otherwise a factor analysis is not useful.
- 2 The sample covariance matrix **S** is an estimate of Σ .

Given the sample and an assumption of non-zero correlations of the components of the observations, how do we estimate the factor loadings l_{ij} and specific variances ψ_i ; keep in mind that the factors F_j for j = 1, ..., m are not observed, so a multivariate regression with the factors as a design matrix is not an option.

We will consider two methods:

- 1 The principal component method
- 2 Maximum likelihood

Principal component method

1 $Y_i = \mathbf{e}_i' \mathbf{X} = e_{i1} X_1 + ... + e_{ip} X_p$ is the i^{th} principal component where \mathbf{e}_i is the i^{th} eigenvector of Σ ; in matrix notation

$$\mathbf{Y} = \mathbf{P}'\mathbf{X}$$
 where $\mathbf{\Sigma} = \mathbf{P}\mathbf{\Lambda}\mathbf{P}'$

- $2 \quad Cov(Y_i, Y_j) = 0$
- 3 PY = PP'X and therefore X = PY

then taking Y as the common factors gets us almost what we want, except $Cov Y = \Lambda$. If we choose instead $L = P\Lambda^{\frac{1}{2}}$ we get

$$\mathbf{\Sigma} = \mathbf{L}\mathbf{L}' + \mathbf{\Psi} = \mathbf{P}\mathbf{\Lambda}^{rac{1}{2}}(\mathbf{P}\mathbf{\Lambda}^{rac{1}{2}})' + \mathbf{0}$$

When $\lambda_{m+1},...,\lambda_p$ are small, we can drop columns $l_{m=1},...,l_p$ from the matrix **L**.

Then

$$oldsymbol{\Sigma} = [\sqrt{\lambda_1} \ \mathbf{e_1}|...|\sqrt{\lambda_m} \ \mathbf{e_m}] \left(egin{matrix} \sqrt{\lambda_1} \ \mathbf{e_1} \ \sqrt{\lambda_2} \ \mathbf{e_2} \ \vdots \ \sqrt{\lambda_m} \ \mathbf{e_m} \end{array}
ight) + \left(egin{matrix} \psi_1 & 0 & \dots & 0 \ 0 & \psi_2 & \dots & 0 \ \vdots & \vdots & \ddots & \vdots \ 0 & 0 & \dots & \psi_m \end{array}
ight)$$

and

$$\psi_i = \sigma_{ii} - \sum_{j=1}^m l_{ij}^2$$

Note:

- 1 Principal components requires all components to account for the total variation and the purpose is to summarize the variability in the observed data.
- 2 Factor analysis accounts for the total variance with only a few common factors (the specific variance accounts for the residual variance not explained by the common factors).

The principal components estimates

- 1 Sample data $\mathbf{x}_1, ..., \mathbf{x}_n$ are p-variate observation vectors with sample covariance matrix \mathbf{S} and correlation matrix \mathbf{R}
- 2 $(\hat{\lambda}_i, \hat{\mathbf{e}}_i)$ for i = 1, ..., p are the eigenvalues and eigenvectors of **S**
- 3 For some m < p we obtain the matrix $\tilde{\mathbf{L}}$ of factor loadings

$$ilde{\mathbf{L}} = ig[\sqrt{\hat{\lambda}_1} \ \hat{\mathbf{e}}_1 \ | \ \sqrt{\hat{\lambda}_2} \ \hat{\mathbf{e}}_2 \ | \ ... \ | \ \sqrt{\hat{\lambda}_m} \ \hat{\mathbf{e}}_mig]$$

and

$$\tilde{\mathbf{\Psi}} = diag(\tilde{\psi}_i)$$
 with $\tilde{\psi} = s_{ii} - \sum_{j=1}^{m} \tilde{l}_{ij}^2$

with communalities

$$\tilde{h}_{i}^{2} = \tilde{l}_{i1}^{2} + \tilde{l}_{i2}^{2} + \dots + \tilde{l}_{im}^{2}$$

4 Note, that **S** is not reproduced with the principal components solution. That would require p factors.

Maximum likelihood

- 1 The **F** and ϵ are assumed jointly normally distributed.
- 2 The observations $\mathbf{X}_j \mu = \mathbf{L}\mathbf{F}'_j + \epsilon_j$ are then also normally distributed.
- 3 The likelihood $L(\mu, \Sigma)$ is expressed as a function of \mathbf{L} and $\mathbf{\Psi}$ through $\mathbf{\Sigma} = \mathbf{L}\mathbf{L}' + \mathbf{\Psi}$. It is maximized subject to the condition $\mathbf{L}'\mathbf{\Psi}^{-1}\mathbf{L} = \mathbf{\Delta}$ where $\mathbf{\Delta}$ is a diagonal matrix; the condition is required to make the MLE's well-defined.
- 4 Note, m the number of factors needs to be chosen prior to obtaining the MLE's.
- 5 The maximum likelihood estimates of the loadings and specific variances are obtained iteratively.
- 6 The maximum likelihood estimates of the commonalities are given by

$$\hat{h}_{i}^{2} = \hat{l}_{i1}^{2} + \hat{l}_{i2}^{2} + \dots + \hat{l}_{im}^{2}$$
 for $i = 1, \dots, p$

Determining the number of factors

1 The test is carried out for the null hypothesis

$$H_0: \ \Sigma_{p \times p} = \mathbf{L}_{p \times m} \mathbf{L}'_{p \times m} + \mathbf{\Psi}_{p \times p}$$

vs the alternative H_1 : Σ is any other symmetric, positive, definite matrix.

2 The test is based on the likelihood ratio statistic

$$-2ln\Lambda = -2ln\left(\frac{|\hat{\mathbf{\Sigma}}|}{|\mathbf{S}_n|}\right)^{-n/2} + n[tr(\hat{\mathbf{\Sigma}}^{-1}\mathbf{S}_n) - p] = nln\left(\frac{|\hat{\mathbf{\Sigma}}|}{|\mathbf{S}_n|}\right)$$

where $\hat{\Sigma} = \hat{\mathbf{L}}\hat{\mathbf{L}}' + \hat{\Psi}$; $\hat{\mathbf{L}}$ and $\hat{\Psi}$ are the maximum likelihood estimates of the factor loadings and the specific factors. Note: $tr(\hat{\Sigma}^{-1}\mathbf{S}_n) - p = 0$ if $\hat{\mathbf{L}}$ and $\hat{\Psi}$ are the MLE's.

3 The degrees of freedom are

$$\nu - \nu_0 = \frac{1}{2}p(p+1) - \left[p(m+1) - \frac{1}{2}m(m-1)\right] = \frac{1}{2}[(p-m)^2 - p - m]$$

4 An improved version of the test was suggested by Bartlett; this test rejects at level α if

$$n-1-\frac{2p+4m+5}{6}ln\frac{|\hat{\mathbf{L}}\hat{\mathbf{L}}'+\hat{\boldsymbol{\Psi}}|}{|\mathbf{S}_n|}.\chi^2_{[(p-m)^2-p-m]/2}(\alpha)$$

- 5 The Bartlett approximation requires that n and n-p are large.
- 6 Since the degrees of freedom must be positive we need

$$m < \frac{1}{2}(2p+1-\sqrt{8p+1})$$

Factor Rotation

Factor loadings are not unique. If $\hat{\mathbf{L}}$ is any estimate of the $p \times m$ matrix of factor loadings, then so is

$$\hat{\mathbf{L}}^* = \hat{\mathbf{L}}\mathbf{T}$$
 where $\mathbf{T}\mathbf{T}' = \mathbf{T}'\mathbf{T} = \mathbf{I}$

so **T** is an orthogonal transformation.

Under such an orthogonal transformation, the estimated covariance matrix remains unchanged, since

$$\hat{\mathbf{L}}\hat{\mathbf{L}}'+\hat{\mathbf{\Psi}}=\hat{\mathbf{L}}\mathbf{T}\mathbf{T}'\mathbf{L}'+\hat{\mathbf{\Psi}}=\hat{\mathbf{L}}^*\hat{\mathbf{L}}^{*\prime}+\hat{\mathbf{\Psi}}$$

Furthermore, the residual matrix remains unchanged, since

$$\mathbf{S}_n - \mathbf{\hat{L}}\mathbf{\hat{L}}' - \mathbf{\hat{\Psi}} = \mathbf{\hat{L}}^*\mathbf{\hat{L}}^{*\prime} - \mathbf{\hat{\Psi}}$$

Therefore, orthogonal rotations do not change the estimate of the covariance matrix. Factor rotation refers to a rotation of the factor loadings to achieve a simpler structure that makes the factors easier to interpret. Ideally, a rotation leads to a structure where each variable loads highly on one factor and has small or moderate loadings on the other factors.

For 2 factors, this rotation can be done visually by inspecting a plot, where the original factors are plotted along perpendicular axis (F_1 is the x-axis, F_2 is the y-axis), the factor loadings \hat{l}_{1i} , \hat{l}_{2i} are plotted for i = 1, ..., p and the axis rotated at an angle ϕ such the rotated factors align more closely with clusters of points.

For more than 2 factors, computational techniques need to be employed. Computer programs such as SAS will do it.

Varimax criterion

Suppose $\tilde{l}_{ij}^* = \hat{l}_{ij}^*/\hat{h}_i$ where \hat{l}_{ij}^* is the rotated coefficient. The (normal) varimax procedure selects the orthogonal transformation that maximizes

$$V = \frac{1}{p} \sum_{j=1}^{m} \left[\sum_{i=1}^{p} \tilde{l}_{ij}^{*4} - \left(\sum_{i=1}^{p} \tilde{l}_{ij}^{*2} \right)^{2} / p \right]$$

After the transformation **T** is determined, the loadings \tilde{l}_{ij}^* are multiplied by \hat{h}_i , so that the original communalities are preserved.

Note: V corresponds to "spreading out" the squares of the loadings on each factor as much as possible. The goal is to find large and negligible coefficients in each column of $\hat{\mathbf{L}}^*$.

One criterion for rotation is the achieve positive and/or negative loadings for each factor.

Thurston (1945, Multiple Factor Analysis), gave the following criteria:

- 1 Each row of $\hat{\mathbf{L}}^*$ should contain at least one zero. The respective factor F is not associated with the component of X represented by that row.
- 2 Each column of $\hat{\mathbf{L}}^*$ should contain at least m zeros. The factor F is not associated with m components of \mathbf{X} .
- 3 Every pair of columns of $\hat{\mathbf{L}}^*$ should contain several components of \mathbf{X} whose loadings vanish in one but not the other. The respective factors load on separate X's.
- 4 If the number of factors is 4 or more, every pair of columns of $\hat{\mathbf{L}}^*$ should contain a large number of components of \mathbf{X} with zero loadings in both columns.
- 5 For every pair of columns of $\hat{\mathbf{L}}^*$ only a small number of components of \mathbf{X} should have nonzero loadings in both columns.

These criteria require that the components of X fall into mutually exclusive groups with loadings high on a single factor and low to moderate on the other factors.

Estimating Factor Scores

- Factor scores are estimates of the unobserved random factors \mathbf{F}_j for j = 1, ..., n; note: \mathbf{X} is the random variable and $\mathbf{x}_1, ..., \mathbf{x}_n$ is a sample from the population; \mathbf{F}_j is the random effect for subject j and $\hat{\mathbf{f}}$ is an estimate of the possible value \mathbf{f}_j of \mathbf{F}_j , \mathbf{F}_j is a subject specific random effect in the same way that ϵ_j is.
- 2 Each subject has 2 random effects associated with it: \mathbf{F}_j and ϵ_j ;
- 3 The relationship is given by

$$\mathbf{X}_{p\times 1} - \mu_{p\times 1} = \mathbf{L}_{p\times m} \mathbf{F}_{m\times 1} + \epsilon_{p\times 1}$$

and both **F** and ϵ are unknown.

4 To estimate \mathbf{f}_j , the following assumptions are made, \hat{l}_{ij} and $\hat{\psi}_i$ are the true values.

The weighted least squares method

1 Factor scores obtained by weighted least squares from the maximum likelihood estimates

$$\hat{\mathbf{f}}_j = (\hat{\mathbf{L}}'\hat{\mathbf{\Psi}}^{-1}\hat{\mathbf{L}})^{-1}\hat{\mathbf{L}}'\hat{\mathbf{\Psi}}^{-1}(\mathbf{x}_j - \hat{\mu})$$

where $\hat{\mathbf{f}}$ is chosen to minimize

$$\epsilon' \mathbf{\Psi}^{-1} \epsilon = (\mathbf{x} - \mu - \mathbf{L}\mathbf{f})' \mathbf{\Psi}^{-1} (\mathbf{x} - \mu - \mathbf{L}\mathbf{f})$$

2 If factor loadings are estimated using the principal components approach, an unweighted least squares method is used to give

$$\mathbf{\hat{f}}_j = \left(ilde{\mathbf{L}}' ilde{\mathbf{L}}
ight)^{-1} ilde{\mathbf{L}}' \left(\mathbf{x}_j - \hat{\mu}
ight)$$

where $\tilde{\mathbf{L}} = \tilde{\mathbf{L}} = \begin{bmatrix} \sqrt{\hat{\lambda}_1} & \hat{\mathbf{e}}_1 & \sqrt{\hat{\lambda}_2} & \hat{\mathbf{e}}_2 & \dots & \sqrt{\hat{\lambda}_m} & \hat{\mathbf{e}}_m \end{bmatrix}$. The estimates are for the covariance matrix; scaled data use $\hat{\mathbf{L}}$ from the correlation matrix.

The regression method

The estimated factor scores are given by

$$\hat{\mathbf{f}}_j = \hat{\mathbf{L}}' \mathbf{S}^{-1} (\mathbf{x}_j - \bar{\mathbf{x}})$$
 $j = 1, ..., n$

Here, **L** and Ψ are treated as known, **F** and ϵ are jointly normal and the joint distribution of $\mathbf{X} - \mu$ and **F** is $N_{p+m}(\mathbf{0}, \Sigma^*)$ with

$$oldsymbol{\Sigma}^* = egin{bmatrix} oldsymbol{\Sigma}_{p imes p} = oldsymbol{\mathbf{L}} oldsymbol{\mathbf{L}}' + oldsymbol{\Psi} & oldsymbol{\mathbf{L}}_{p imes m} \ oldsymbol{\mathbf{L}}'_{m imes p} & oldsymbol{\mathbf{I}}_{m imes m} \end{bmatrix}$$

then

$$E(\mathbf{F} \mid \mathbf{x}) = \mathbf{L}' \mathbf{\Sigma}^{-1} (\mathbf{x} - \mu) = \mathbf{L}' (\mathbf{F} \mathbf{F}' + \mathbf{\Psi})^{-1} (\mathbf{x} - \mu)$$

and we substitute the maximum likelihood estimates of $\hat{\mathbf{L}}$, $\hat{\boldsymbol{\Psi}}$ and μ ; finally, \mathbf{S} is substituted for $\hat{\mathbf{F}}\hat{\mathbf{F}}' + \hat{\boldsymbol{\Psi}}$

Strategy for Factor Analysis

- 1 Perform a principal component factor analysis, ie use principal component approach to obtain factors.
 - a. look for suspicious observations using methods for multivariate normal data
 - b. try varimax rotation
- 2 Perform maximum likelihood factor analysis (use a computer program for that), including varimax rotation
- 3 Compare the solutions
- 4 Repeat the steps with different m.
- 5 If data set is large split into two data sets and perform factor analysis on each set; compare results
- 6 Consult with an expert in the field the data was collected for. If they think the results are non-informative, try again.