

## Displays for Statistics 5401/8401

## Lecture 29

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Class Web Page

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There are two important and different types of factor analysis - **exploratory factor analysis** and **confirmatory factor analysis**.

**Exploratory factor analysis** estimates the factor analysis model with some purely mathematical restriction (e.g.  $L'L$  diagonal) on the loading matrix  $L$  to assure uniqueness. Then  $\hat{L}$  is "rotated" to have an "interpretable" structure.

For example a rotated  $\hat{L}$  might be

$$\hat{L} = \begin{matrix} & f_1 & f_2 \\ x_1 & \begin{bmatrix} .99 & -.08 \end{bmatrix} \\ x_2 & \begin{bmatrix} -.10 & -.81 \end{bmatrix} \\ x_3 & \begin{bmatrix} .09 & .58 \end{bmatrix} \end{matrix} \approx \begin{bmatrix} 1 & 0 \\ 0 & -.8 \\ 0 & .6 \end{bmatrix}$$

**Interpretation:**

- $x_1$  is affected only by factor 1
- $x_2$  and  $x_3$  are affected only by factor 2.

You use **confirmatory factor analysis** with a pre-determined form for  $\mathbf{L}$  like

$$\mathbf{L} = \begin{bmatrix} * & 0 \\ 0 & * \\ 0 & * \end{bmatrix} \quad (* \text{ means non-zero})$$

The pattern might come from an earlier exploratory factor analysis or from subject-matter knowledge.

You estimate  $\mathbf{L}$  by finding the best fitting loadings *of this form*, that is with  $l_{12} = l_{21} = l_{31} = 0$ .

A goodness-of-fit test of  $\hat{\Sigma} = \hat{\mathbf{L}}\hat{\mathbf{L}}' + \hat{\Psi}$  to  $\mathbf{S}$  or  $\hat{\rho}$  to  $\mathbf{R}$  tests the null hypothesis

$$H_0: l_{12} = l_{21} = l_{31} = 0$$

vs

$$H_1: \text{no special pattern of 0's.}$$

When you cannot reject  $H_0$ , then the proposed pattern is *confirmed*.

Confirmatory factor analysis is a special case of **structural equation modeling**.

My focus is on exploratory factor analysis.

### Recapitulate

The factor analytic model for  $\mathbf{x}$  is

$$\mathbf{x} = \boldsymbol{\mu} + \mathbf{L}\mathbf{f} + \boldsymbol{\varepsilon}.$$

$\Sigma = V[\mathbf{X}]$  has the factor analytic form

$$\Sigma = \underset{\text{rank } m}{\mathbf{V}} + \underset{\text{diagonal}}{\Psi} = \mathbf{L}\mathbf{\Gamma}\mathbf{L}' + \Psi, \mathbf{\Gamma} = V[\mathbf{f}]$$

where

- $\Psi = \text{Var}[\boldsymbol{\varepsilon}] = \text{diag}[\psi_1, \psi_2, \dots, \psi_p]$  is  $p$  by  $p$  diagonal with  $\psi_i \geq 0$
- $\mathbf{L}$  is  $p$  by  $m$
- $\mathbf{\Gamma} = V[\mathbf{f}]$  is  $m$  by  $m$
- $\mathbf{V} = \mathbf{L}\mathbf{\Gamma}\mathbf{L}'$  has rank  $m < p$

Only  $\mathbf{V}$  and  $\Psi$  are uniquely defined. Given  $\mathbf{V}$  and  $\Psi$ , there are infinitely many  $p$  by  $m$   $\mathbf{L}$  and  $m$  by  $m$   $\mathbf{\Gamma}$  with  $\mathbf{V} = \mathbf{L}\mathbf{\Gamma}\mathbf{L}'$ .

$\mathbf{\Gamma} = \mathbf{I}_m$  characterizes the orthogonal factor model.

Exploratory factor analysis usually consists of two phases

- 1 *Factor extraction* - compute estimates  $\hat{\Psi}$  and  $\hat{\mathbf{V}} = \hat{\mathbf{L}}\hat{\mathbf{L}}'$ , where  $\hat{\mathbf{L}}$  satisfies a mathematical restriction to achieve uniqueness and may not be interpretable.

This is followed by

- 2 *Factor rotation* - modifies  $\hat{\mathbf{L}}$  without changing  $\hat{\mathbf{V}} = \hat{\mathbf{L}}\hat{\mathbf{L}}'$  so as to try to achieve an interpretable form for  $\hat{\mathbf{L}}$ .

With oblique factor analysis,  $\hat{\mathbf{\Gamma}}$  and  $\hat{\mathbf{L}}$  are found so that  $\hat{\mathbf{V}} = \hat{\mathbf{L}}\hat{\mathbf{\Gamma}}\hat{\mathbf{L}}'$  and  $\hat{\mathbf{L}}$  has interpretable structure and  $\hat{\mathbf{\Gamma}}$  provides information about how the factors are related. You can often get a "simpler"  $\hat{\mathbf{L}}$  than with  $\mathbf{\Gamma} = \mathbf{I}_m$ .

You start with the sample variance matrix  $\mathbf{S}$  or correlation matrix  $\mathbf{R}$ .

Usually

$$\mathbf{S} = (n-1)^{-1} \sum_{1 \leq i \leq n} (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})'$$

comes from a random sample  $\mathbf{x}_1, \dots, \mathbf{x}_n$ .

$\mathbf{S}$  can also be a "pooled" matrix

$$\mathbf{S} = f_e^{-1} \mathbf{E}$$

where  $\mathbf{E}$  is the error matrix from a MANOVA or MANACOVA.

The estimated correlation matrix is

$$\mathbf{R} = \mathbf{DSD}$$

with

$$\mathbf{D} = \text{diag}[1/\sqrt{s_{11}}, 1/\sqrt{s_{22}}, \dots, 1/\sqrt{s_{pp}}].$$

For two methods of estimation, GLS and MLE (but not ULS), you get essentially the same results whether you start with  $\mathbf{S}$  or  $\mathbf{R}$ . This contrasts strongly with Principal Components Analysis.

In **covariance-based factor extraction** you try to approximate  $\mathbf{S}$  by finding

$$p \text{ by } m \hat{\mathbf{L}} \text{ and diagonal } p \text{ by } p \hat{\Psi}$$

such that

$$[\hat{\sigma}_{ij}] = \hat{\Sigma} \equiv \hat{\mathbf{L}}\hat{\mathbf{L}}' + \hat{\Psi} = \hat{\mathbf{V}} + \hat{\Psi} \approx \mathbf{S}$$

When the factor analytic model is correct,  $\hat{\Sigma}$  will be a "better" estimate of  $\Sigma$  than  $\mathbf{S}$ , because  $\hat{\Sigma}$  has factor analytic structure while  $\mathbf{S}$  does not.

**Correlation-based** factor analysis tries to approximate

$$\mathbf{R} = \begin{bmatrix} 1 & r_{12} & r_{13} & \dots & r_{1p} \\ r_{21} & 1 & r_{23} & \dots & r_{2p} \\ \dots & \dots & \dots & \dots & \dots \\ r_{p1} & r_{p2} & \dots & r_{p,p-1} & 1 \end{bmatrix}, r_{ij} = r_{ji}$$

by a matrix of the form  $\hat{\rho} \equiv \hat{\mathbf{L}}\hat{\mathbf{L}}' + \hat{\Psi}$  which should be a better estimator of  $\rho$  than  $\mathbf{R}$ .

Usually factor analysis starts with  $\mathbf{R}$ . Because  $\hat{\mathbf{V}} = \hat{\mathbf{L}}\hat{\mathbf{L}}'$  appears in the approximations for  $\Sigma$  and  $\rho$ , the factor extraction phase is based on an orthogonal factor model, but this is only for mathematical convenience.

Finding  $\hat{\mathbf{L}}$  in this phase is just the way you find the rank  $m$  piece  $\hat{\mathbf{V}} = \hat{\mathbf{L}}\hat{\mathbf{L}}'$  of the factor analytic estimate  $\hat{\Sigma} = \hat{\mathbf{V}} + \hat{\Psi}$  or  $\hat{\rho} = \hat{\mathbf{V}} + \hat{\Psi}$ .

I will focus on methods starting with  $\mathbf{S}$ . They can be applied to  $\mathbf{R}$  by substituting  $\rho$  and  $\mathbf{R}$  for  $\Sigma$  and  $\mathbf{S}$  in what follows.

The most usual mathematical restrictions on  $\hat{L}$  are

- $\hat{L}'\hat{L}$  is diagonal (columns of  $\hat{L}$  are orthogonal), assumed for **ULS** (unweighted least squares) estimation
- $\hat{L}'\hat{\Psi}^{-1}\hat{L}$  is diagonal (columns of  $\hat{\Psi}^{-1/2}\hat{L}$  are orthogonal), assumed for **GLS** (generalized least squares) and **MLE** (maximum likelihood) estimation.

Neither restriction on  $\hat{L}$  appears to have an interpretable meaning.

Both are particular cases (when  $\mathbf{Q} = \mathbf{I}_p$  and  $\mathbf{Q} = \hat{\Psi}$ ) of

- $\mathbf{L}'\mathbf{Q}^{-1}\mathbf{L}$  is diagonal
- $\mathbf{Q}$  positive definite, possibly depending on  $\hat{\Psi}$ .

**Fact:**

Suppose you have found  $\hat{V}$  by some means or other. Then you can find  $\hat{L}_Q$  such that  $\hat{V} = \hat{L}_Q\hat{L}_Q'$  and  $\hat{L}_Q$  satisfies

$$\hat{L}_Q'\mathbf{Q}^{-1}\hat{L}_Q \text{ is diagonal}$$

where  $\mathbf{Q}$  is a specific positive definite symmetric matrix, say  $\hat{\Psi}$ .

$$\hat{L}_Q = [\hat{\ell}_{1Q}, \dots, \hat{\ell}_{mQ}], \quad \hat{\ell}_{iQ} = \sqrt{\delta_i} \mathbf{Q} \mathbf{e}_i$$

where

- $\mathbf{e}_1, \dots, \mathbf{e}_m$  are the first  $m$  eigenvectors of  $\hat{V}$  relative to  $\mathbf{Q}$
- $\delta_1, \dots, \delta_m$  the first  $m$  relative eigenvalues

With this choice  $\hat{V} = \hat{L}_Q\hat{L}_Q'$  and

$$\hat{L}_Q'\mathbf{Q}^{-1}\hat{L}_Q = \text{diag}[\delta_1, \delta_2, \dots, \delta_m]$$

is diagonal.

1. Diagonal  $\hat{\mathbf{L}}'\hat{\mathbf{L}}$  corresponds to  $\mathbf{Q} = \mathbf{I}_p$  when relative eigenvalues and vectors are ordinary eigenvalues  $\hat{\lambda}_i$  and eigenvectors  $\hat{\mathbf{v}}_i$  of  $\hat{\mathbf{V}}$ , so the columns of  $\hat{\mathbf{L}}$  are  $\hat{\mathbf{l}}_j = \sqrt{\hat{\lambda}_i} \hat{\mathbf{v}}_i$ .
2. Diagonal  $\hat{\mathbf{L}}'\hat{\Psi}^{-1}\hat{\mathbf{L}}$  corresponds to  $\mathbf{Q} = \hat{\Psi}$ . In this case  $\hat{\mathbf{l}}_j = \sqrt{\delta_i} \mathbf{u}_i$ , where  $\delta_i$  and  $\mathbf{u}_i$  are eigenvalue and eigenvector of  $\hat{\mathbf{V}}$  *relative* to  $\hat{\Psi}$ .

We will look at several ways to estimate  $\mathbf{V}$ , including the ULS, GLS and MLE (or ML) methods

ULS assumes  $\mathbf{L}'\mathbf{L}$  is diagonal ( $\mathbf{Q} = \mathbf{I}_p$ ).

GLS and ML assumes  $\mathbf{L}'\Psi^{-1}\mathbf{L}$  is diagonal ( $\mathbf{Q} = \Psi$ ).

To summarize exploratory factor analysis:

**Phase 1: *Extraction*:**

$$(\mathbf{x}_1, \dots, \mathbf{x}_n) \rightarrow (\mathbf{S} \text{ or } \mathbf{R}) \rightarrow (\hat{\mathbf{L}}, \hat{\Psi}) \rightarrow (\hat{\mathbf{V}}, \hat{\Psi}),$$

$$\hat{\mathbf{V}} = \hat{\mathbf{L}}\hat{\mathbf{L}}'$$

where  $\hat{\mathbf{L}}$  satisfies a mathematical restriction that makes it unique.

**Phase 2: *Rotation*:**

Find  $\mathbf{H}$  (and possibly  $\hat{\Gamma}$ ) so that

$$\hat{\mathbf{L}}^* = \hat{\mathbf{L}} \mathbf{H} \text{ is interpretable}$$

with  $\hat{\mathbf{V}} = \hat{\mathbf{L}}^* \hat{\mathbf{L}}^{*'} , (\text{or } \hat{\mathbf{V}} = \hat{\mathbf{L}}^* \hat{\Gamma} \hat{\mathbf{L}}^{*'})$

The choice of  $\hat{\mathbf{L}}^*$  (or  $\mathbf{H}$ ) must be based on substantive scientific reasons, not mathematical convenience.

All methods of rotation share the idea of finding  $\mathbf{H}$  so that  $\hat{\mathbf{L}}^* = \hat{\mathbf{L}}\mathbf{H}$  has *simple structure*.

The left matrix is "not simple" (\* means non-zero); the right matrix would generally be considered simpler

$$\hat{\mathbf{L}} = \begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}, \hat{\mathbf{L}}^* = \begin{bmatrix} * & 0 & 0 \\ * & 0 & 0 \\ * & * & 0 \\ 0 & * & 0 \\ 0 & 0 & * \end{bmatrix}$$

- In  $\hat{\mathbf{L}}$  all  $p = 5$  variables load on all  $m = 3$  factors. This is not simple.
- In  $\hat{\mathbf{L}}^*$ , variables  $x_1$  and  $x_2$  load *only* on  $f_1$ ,  $x_3$  loads on  $f_1$  *and*  $f_2$ ,  $x_4$  loads *only* on  $f_2$ , and  $x_5$  loads *only* on  $f_3$ . And factor  $f_1$  affects only  $x_1$ ,  $x_2$  and  $x_3$ ,  $f_2$  affects only  $x_3$  and  $x_4$ , and  $f_3$  affects only  $x_5$ .

The simpler pattern *might* be more interpretable *by a subject matter expert*, especially if you can identify a feature that is shared by  $x_1$  and  $x_2$ .

For example, if both  $x_1$  and  $x_2$  were concerned with a subject's logical thinking skills, then it *might* be possible to identify  $f_1$  as a "clear thinking" factor. You would need subject matter knowledge to do this with confidence.

Most computational rotation methods such as *varimax* and *quartimax* find  $\mathbf{H}$

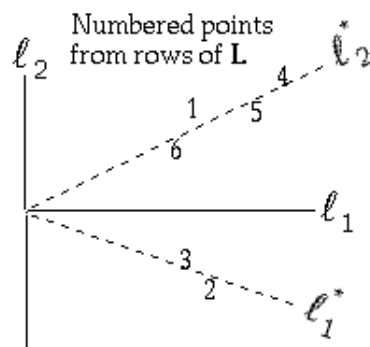
- to *maximize*  $I_s(\hat{\mathbf{L}}\mathbf{H})$  where  $I_s(\mathbf{L})$  is a "simplicity" index
- or to *minimize*  $I_c(\hat{\mathbf{L}}\mathbf{H})$ , where  $I_c(\mathbf{L})$  is a "complexity" index.

For varimax and quartimax the criterion function is a degree 4 polynomial in  $\ell_{ij}$ .

For oblique (non-orthogonal) factor rotation, you "rotate" with a matrix  $H$  that is not a rotation matrix, that is  $H'H \neq I_m$  and  $\Gamma = V[f] \neq I_m$ .

Here is an  $m = 2$  example when this might be appropriate. No *orthogonal* rotation will produce simple form.

Using coordinates based on the non perpendicular dashed lines, variables 3 and 2 will load primarily on factor 1 and variables 1, 4, 5, and 6 on factor 2, a simple structure.



That is,  $L^*$  has the form

$$L^* = \begin{bmatrix} 0 & * \\ * & 0 \\ * & 0 \\ 0 & * \\ 0 & * \\ 0 & * \end{bmatrix}$$

The rotated factors  $f_j^*$  will *not* be uncorrelated ( $\Gamma$  not diagonal).

We will look at four or five methods of factor extraction:

- PC = Principal Components
- IPF = Iterated principal factor
- ULS = Unweighted Least Squares
- GLS = Generalized Least Squares
- ML = Maximum likelihood assuming normality.

All except PC require iteration.

IPF is sometimes an option on computer programs. It is a simple iterative method that should lead to the same solution as the ULS method. IPF is generally not recommended because it may need a huge number of steps. There are similar inferior iterative methods for GLS and MLE.

ULS, GLS and MLE estimates each attempt to minimize a specific criterion which measures the discrepancy between  $S$  (or  $R$ ) and the estimate  $\hat{\Sigma} = \hat{L}\hat{L}' + \hat{\Psi}$ .



## Principal Component Factor Estimation

The PC method approximates  $\mathbf{x}$  in terms of the first few sample principal components  $\hat{z}_j = \hat{\mathbf{v}}_j'(\mathbf{x} - \bar{\mathbf{x}})$

### Summary of method

- Find the eigenvectors  $\hat{\mathbf{v}}_j$  and eigenvalues  $\hat{\lambda}_j$ ,  $j = 1, \dots, p$  of the sample covariance matrix  $\mathbf{S}$  or (more usually) the sample correlation matrix  $\mathbf{R}$ .
- For a suitable choice of  $m$  (usually the number of eigenvalues greater than a threshold such as 1), the *unrotated* estimated loading matrix is

$$\begin{aligned} \hat{\mathbf{L}} &= [\sqrt{\hat{\lambda}_1} \hat{\mathbf{v}}_1, \dots, \sqrt{\hat{\lambda}_m} \hat{\mathbf{v}}_m] \\ &= [\hat{\boldsymbol{\ell}}_1, \dots, \hat{\boldsymbol{\ell}}_m], \quad \hat{\ell}_{ij} = \sqrt{\hat{\lambda}_j} \times \hat{v}_{ij} \end{aligned}$$

Because eigenvectors are orthonormal,  $\hat{\mathbf{L}}'\hat{\mathbf{L}} = \text{diag}[\hat{\lambda}_1, \dots, \hat{\lambda}_m]$  is diagonal.

- The estimated factors are  $\hat{f}_j = \hat{z}_j / \sqrt{\hat{\lambda}_j}$

- You estimate  $\mathbf{V}$  by  $\hat{\mathbf{V}} = \hat{\mathbf{L}}\hat{\mathbf{L}}'$ .  $\hat{\mathbf{V}}$  is the best (least squares) rank  $m$  approximation to  $\mathbf{S}$  (or  $\mathbf{R}$ ).
- You find  $\hat{\boldsymbol{\Psi}}$  so that the diagonal of  $\hat{\boldsymbol{\Sigma}} = \hat{\mathbf{L}}\hat{\mathbf{L}}' + \hat{\boldsymbol{\Psi}}$  *exactly matches* the diagonal of  $\mathbf{S}$ . That is

$$\hat{\boldsymbol{\Psi}} = \text{diag}[\mathbf{S} - \hat{\mathbf{L}}\hat{\mathbf{L}}'], = \text{diag}[\mathbf{S} - \hat{\mathbf{V}}]$$

or explicitly

$$\hat{\psi}_i = s_{ii} - \sum_{1 \leq j \leq m} \hat{\ell}_{ij}^2, \quad i = 1, \dots, p.$$

The estimated communalities are

$$\hat{h}_i^2 = s_{ii} - \hat{\psi}_i = \sum_{1 \leq j \leq m} \hat{\ell}_{ij}^2.$$

When  $\mathbf{S} = \mathbf{R}$ ,  $\hat{h}_i^2 = 1 - \hat{\psi}_i$

*Notation note:*

When  $\mathbf{A} = [a_{ij}]$ , the notation  $\text{diag}[\mathbf{A}]$  means the diagonal matrix  $\text{diag}[a_{11}, \dots, a_{pp}]$ .

### Example: Artificial data with $m = 2$

```
Cmd> s <- tabs(y,covar:T); s # sample variance matrix
(1,1) 3.1903 0.6777 -2.2794 -0.62891 0.71555
(2,1) 0.6777 1.3874 -1.2398 -0.3807 0.29635
(3,1) -2.2794 -1.2398 7.7395 1.7365 -1.8761
(4,1) -0.62891 -0.3807 1.7365 0.73894 -0.56029
(5,1) 0.71555 0.29635 -1.8761 -0.56029 0.87565
```

```
Cmd> eigs <- eigen(s)
```

```
Cmd> eigs$values # eigenvalues of S
(1) 9.8495 2.2704 1.1149 0.46384 0.23323
```

```
Cmd> m <- 2
```

```
Cmd> Lhat <- sqrt(eigs$values[run(m)]') * eigs$ectors[,run(m)]
```

```
Cmd> Lhat # unrotated estimated loadings
(1,1) 1.1223 1.3747
(2,1) 0.54182 0.19703
(3,1) -2.7107 0.57841
(4,1) -0.66079 0.062869
(5,1) 0.71535 -0.056138
```

Columns  
are  
 $\sqrt{\hat{\lambda}_j} \hat{\mathbf{v}}_j$

```
Cmd> psihat <- diag(s) - diag(Lhat %** L'); psihat
(1) 0.040853 1.055 0.056965 0.29834 0.36078
```

These are the estimated uniquenesses  $\hat{\psi}_j$ .

```
Cmd> Vhat <- Lhat %** Lhat'; Vhat # rank 2 piece
(1,1) 3.1495 0.87894 -2.247 -0.65517 0.72565
(2,1) 0.87894 0.33239 -1.3547 -0.34564 0.37653
(3,1) -2.247 -1.3547 7.6826 1.8276 -1.9716
(4,1) -0.65517 -0.34564 1.8276 0.44059 -0.47622
(5,1) 0.72565 0.37653 -1.9716 -0.47622 0.51488
```

```
Cmd> h <- diag(vhat); h #c Estimated omunalities
(1) 3.1495 0.33239 7.6826 0.44059 0.51488
```

```
Cmd> sigmahat <- Vhat + dmat(psihat)
```

```
Cmd> sigmahat # Estimated variance matrix;diags exactly match S
(1,1) 3.1903 0.87894 -2.247 -0.65517 0.72565
(2,1) 0.87894 1.3874 -1.3547 -0.34564 0.37653
(3,1) -2.247 -1.3547 7.7395 1.8276 -1.9716
(4,1) -0.65517 -0.34564 1.8276 0.73894 -0.47622
(5,1) 0.72565 0.37653 -1.9716 -0.47622 0.87565
```

### Advantages of PC factor estimation

- Estimated uniqueness  $\hat{\psi}_i$  and unrotated loadings  $\hat{\mathbf{L}}$  are explicit functions of eigenvalues and eigenvectors of  $\mathbf{S}$  or  $\mathbf{R}$ . *No iteration is required.*
- You can obtain loadings for any  $m \leq p$
- $\hat{\mathbf{l}}_j$  doesn't change when  $m$  changes.

### Disadvantage:

- The PC method does not actually estimate either  $\mathbf{\Psi}$  or  $\mathbf{V} = \mathbf{L}\mathbf{L}'$ .

Even when  $\mathbf{\Sigma} = \mathbf{V} + \mathbf{\Psi}$  and  $\mathbf{S} = \mathbf{\Sigma}$ , the principal component method does not reproduce  $\mathbf{V}$  and  $\mathbf{\Psi}$ . This is because in the Principal Component "model"

$$\mathbf{x} = \boldsymbol{\mu} + \sum_{1 \leq j \leq m} f_j \mathbf{l}_j + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} = \sum_{m+1 \leq j \leq p} z_j \mathbf{v}_j$$

$$f_j = z_j / \sqrt{\lambda_j}, \mathbf{l}_j = \sqrt{\lambda_j} \mathbf{v}_j.$$

But  $V[\boldsymbol{\varepsilon}] = \sum_{m+1 \leq j \leq p} \lambda_j \mathbf{v}_j \mathbf{v}_j'$  is *not* diagonal.

## Iterated Principal Factor Estimation

The *iterated principal factor* (IPF) method of factor extraction is iterative. Each step or stage is quite similar to the PC method.

At the  $i^{\text{th}}$  stage you have a trial value  $\hat{\Psi}_{(i)}$ . If  $\hat{\Psi}_{(i)}$  is close to the true  $\Psi$  then  $\mathbf{V}^* = \mathbf{S} - \hat{\Psi}_{(i)}$  should be close to the true rank  $m$  matrix  $\mathbf{V}$ .

Then you find a  $p$  by  $m$   $\hat{\mathbf{L}}_{(i+1)}$  such that  $\hat{\mathbf{V}}_{(i+1)} = \hat{\mathbf{L}}_{(i+1)} \hat{\mathbf{L}}_{(i+1)}'$  is the best rank  $m$  approximation to  $\mathbf{V}_{(i)}^* \equiv \mathbf{S} - \hat{\Psi}_{(i)}$ .

But this is

$$\hat{\mathbf{L}}_{(i+1)} = [\sqrt{\delta_1} \mathbf{e}_1, \dots, \sqrt{\delta_m} \mathbf{e}_m].$$

where  $\delta_j$  and  $\mathbf{e}_j$  are the eigenvalues and eigenvectors of  $\mathbf{V}_{(i)}^*$ . This is like the PC method but with  $\mathbf{V}_{(i)}^*$  replacing  $\mathbf{S}$ .

Because the eigenvectors  $\mathbf{e}_j$  are orthonormal,  $\hat{\mathbf{L}}_{(i+1)}' \hat{\mathbf{L}}_{(i+1)} = \text{diag}[\delta_1, \dots, \delta_m]$  and thus is diagonal.

You then get a new  $\hat{\Psi}$  as

$$\hat{\Psi}_{(i+1)} = \text{diag}[\mathbf{S} - \hat{\mathbf{L}}_{(i+1)} \hat{\mathbf{L}}_{(i+1)}']$$

just as in the PC method.

To summarize: At the  $i^{\text{th}}$  iteration:

- $\hat{\Psi}_{(i)}$  and  $\hat{\mathbf{L}}_{(i)}$  are current trial values.
- $\hat{\Sigma}_{(i)} = \hat{\mathbf{L}}_{(i)} \hat{\mathbf{L}}_{(i)}' + \hat{\Psi}_{(i)} = \hat{\mathbf{V}}_{(i)} + \hat{\Psi}_{(i)}$  is the current approximation to  $\mathbf{S}$  based on  $\hat{\Psi}_{(i)}$  and  $\hat{\mathbf{L}}_{(i)}$ .

After iteration  $i+1$

- $\hat{\mathbf{L}}_{(i+1)} = [\sqrt{\delta_1} \mathbf{e}_1, \dots, \sqrt{\delta_m} \mathbf{e}_m]$ ,  $\delta_j$  and  $\mathbf{e}_j$  eigenvalues and vectors of  $\mathbf{V}_{(i)}^* = \mathbf{S} - \hat{\Psi}_{(i)}$
- $\hat{\Psi}_{(i+1)} = \text{diag}[\mathbf{S} - \hat{\mathbf{L}}_{(i+1)} \hat{\mathbf{L}}_{(i+1)}']$ .

Substitute  $\mathbf{R}$  for  $\mathbf{S}$  when working with correlations.

You continue the iteration until it converges (if it does), that is,

$$\hat{\Psi}_{(i+1)} - \hat{\Psi}_{(i)} \approx \mathbf{0} \text{ or } \hat{\Sigma}_{(i+1)} - \hat{\Sigma}_{(i)} \approx \mathbf{0}.$$

In practice, it may converge very slowly. Or it can abort if at some point  $\delta_m < 0$  so that  $\sqrt{\delta_m}$  can't be calculated.

Note:

- At each stage,  $\hat{\Psi}_{(i)}$  is *all* you need to go to the next stage, since the next stage is computed from the eigenvalues and vectors of  $\mathbf{V}^* = \mathbf{S} - \hat{\Psi}_{(i)}$ .
- To start the iteration, you must provide an *initial value*  $\hat{\Psi}_{(0)}$  for  $\Psi$ .

The most usual is

$$\hat{\Psi}_{(0)} = \text{diag}[1/s^{11}, 1/s^{22}, \dots, 1/s^{pp}]$$

where  $\mathbf{S}^{-1} = [s^{kk}]$ .

$1/s^{kk}$  is essentially  $1 - R^2$  in a regression of  $x_k$  on the other  $x$ 's.