Factor Loading Recovery for Smoothed Tetrachoric Correlation Matrices

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Introduction

Overview

We often want to conduct exploratory factor analysis on binary response data

- The assumption of continuous outcomes required by the common linear factor model is violated when data are binary
- Tetrachoric correlation matrices (Brown & Benedetti, 1977; Divgi, 1979) are often used to estimate the correlations between the normally-distributed, continuous latent variables often assumed to underlie observed binary data
- Tetrachoric correlation matrices are sometimes indefinite
- Matrix smoothing algorithms produce a proper “smoothed” matrix from and indefinite matrix

Previous Work

- Knol & Berger (1991) found no significant differences between factor solutions from smoothed and unsmoothed (indefinite) tetrachoric correlation matrices
    - Very small study; 10 indefinite correlation matrices with 250 subjects and 15 items
- Debelak & Tran (2013) and Debelak & Tran (2016): Smoothed vs. unsmoothed tetrachoric correlation matrices for parallel analysis
    - Smoothing improved dimensionality recovery (best results for Bentler-Yuan)
    - Differences were small
- Kracht and Waller (under review): Smoothed tetrachoric correlation matrices for parallel analysis
    - Only slight differences between smoothing algorithms
    - Bentler-Yuan led to slightly better results in some conditions

1. Are smoothed matrices better approximations of their corresponding population correlation matrices than indefinite tetrachoric correlation matrices?
2. When used in factor analysis, do smoothed correlation matrices lead to better factor loading estimates than indefinite tetrachoric correlation matrices?
3. Do three commonly-used smoothing algorithms differ with respect to Questions (1) and (2)?
    - Higham (2002)
    - Bentler-Yuan (2011)
    - Knol-Berger (1991)

Background

Proper Correlation Matrices

By definition, a proper correlation matrix, $\mathbf{R}_{p\times p} = \{r_{ij}\}$, satisfies:

- $r_{ij} = r_{ji}$ (symmetry)
- $\mathrm{diag}(\mathbf{R}) = \mathbf{I}$ (unit diagonal)
- $r_{ij} \in [-1, 1]$ (elements bounded by -1 and 1)
- $\mathbf{R} \succcurlyeq 0$ (positive semidefinite)

The Problem with Indefinite Correlation Matrices

$\mathbf{R}_{\text{tet}}$: The tetrachoric correlation matrix

$\mathbf{R}_{\text{Pop}}$: The population correlation matrix estimated by $\mathbf{R}_{\text{tet}}$

Problems:

- An indefinite $\mathbf{R}_{\text{tet}}$ is not in the set of possible $\mathbf{R}_{\text{Pop}}$ matrices
- Some multivariate analysis procedures require PSD correlation matrices (i.e., maximum likelihood factor analysis)
- Can lead to nonsensical interpretations (e.g., negative component variance in PCA)

A matrix smoothing algorithm is a procedure that modifies an indefinite correlation matrix to produce a correlation matrix that is at least PSD.

- The Higham Alternating Projections algorithm (APA; Higham, 2002)
- The Bentler-Yuan algorithm (BY; Bentler & Yuan, 2011)
- The Knol-Berger algorithm (KB; Knol & Berger, 1991)

The Higham Alternating Projections Algorithm (2002)

Intuition: Find the closest PSD correlation matrix ($\mathbf{R}_{\text{APA}}$) to a given indefinite correlation matrix ($\mathbf{R}_{\_}$) by iteratively projecting between two sets:

- $\mathcal{S}$: The set containing all possible $p \times p$ symmetric matrices that are PSD
- $\mathcal{U}$: The set containing all possible $p \times p$ symmetric matrices that have a unit diagonal

For symmetric matrix $\mathbf{A} \in \mathbb{R}^{p \times p}$, define two projection functions:

- $P_S(\mathbf{A}) = \mathbf{V}\mathrm{diag}(\max(\lambda_i, 0))\mathbf{V}'$: Project $\mathbf{A}$ onto $\mathcal{S}$ by replacing all negative eigenvalues with zero in the eigendecomposition.
- $P_U(\mathbf{A})$: Project $\mathbf{A}$ onto $\mathcal{U}$ by replacing the diagonal elements of $\mathbf{A}$ with ones.

The Higham Alternating Projections Algorithm (2002)

Initialize $\mathbf{A}_0$ as the indefinite correlation matrix $\mathbf{R}\_$. Repeat the operation

$$\mathbf{A}_{k+1} = P_U(P_S(\mathbf{A}_k))$$

until convergence occurs or the maximum number of iterations is exceeded.

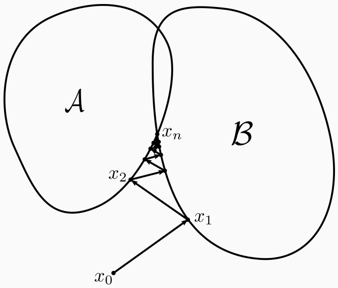


Figure 1: Simplified illustration of the method of alternating projections.

The Bentler-Yuan Algorithm (2011)

Intuition: Shrink the correlations involving variables with minimum trace factor analysis (MTFA; Jamshidian & Bentler, 1998) estimated communalities ≥ 1.

$$\mathbf{R}_{\mathrm{BY}} = \Delta \mathbf{R}_0 \Delta + \mathbf{I}$$

$\mathbf{R}_0 = \mathbf{R}\_ - \mathbf{I}$
Δ^2 is a diagonal matrix with elements δ_i^2,

$$\delta_i^2 = \begin{cases} 1 & \text{if } h_i < 1 \\ k/h_i & \text{if } h_i \geq 1. \end{cases}$$

$k \in (0,1)$ is a constant chosen by the user
h_i is the MTFA communality estimate for the ith item

The Knol-Berger Algorithm (1991)

Intuition: Replace all negative eigenvalues with a small non-negative constant in the eigenvalue decomposition and then scale the result to a correlation matrix.

The Knol-Berger Algorithm (1991)

$$\mathbf{R}_{\_} = \mathbf{V}\Lambda\mathbf{V}'$$

$$\Lambda_{+} = \mathsf{diag}[\mathsf{max}(\lambda_i, 0)],\ i \in \{1, \ldots, p\}$$

$$\mathbf{R}_{\mathrm{KB}} = [\mathrm{dg}(\mathbf{V}\Lambda_{+}\mathbf{V}')]^{-1/2}\mathbf{V}\Lambda_{+}\mathbf{V}'[\mathrm{dg}(\mathbf{V}\Lambda_{+}\mathbf{V}')]^{-1/2}$$

$$\mathbf{R}_{\_} = \begin{bmatrix} 1 & 0.48 & 0.64 & 0.48 & 0.65 & 0.83 \\ 0.48 & 1 & 0.52 & 0.23 & 0.68 & 0.75 \\ 0.64 & 0.52 & 1 & 0.60 & 0.58 & 0.74 \\ 0.48 & 0.23 & 0.60 & 1 & 0.74 & 0.80 \\ 0.65 & 0.68 & 0.58 & 0.74 & 1 & 0.80 \\ 0.83 & 0.75 & 0.74 & 0.80 & 0.80 & 1 \end{bmatrix}$$

Eigenvalues: (4.21, 0.77, 0.52, 0.38, 0.18, -0.06)

Communalities: (1.029, 1.122, 0.557, 1.299, 0.823, 0.997)

Variables 1, 2, and 4 have estimated communalities > 1.

Example: Matrix Smoothing Algorithms

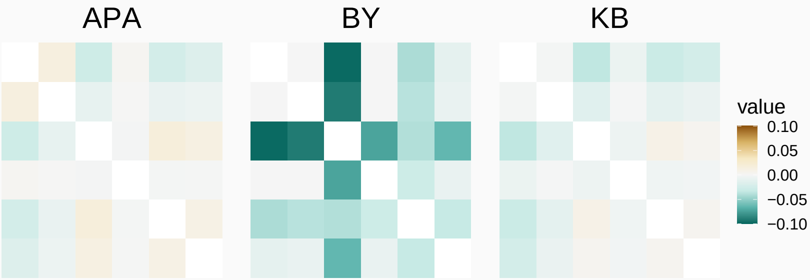


Figure 2: Differences between the elements of the $\mathbf{R}_{\mathrm{Sm}}$ and $\mathbf{R}_{\_}$ matrices for the Higham, Bentler-Yuan, and Knol-Berger algorithms.

Common Factor Model with Model Approximation Error

Tucker et al. (1969)

$$\mathbf{P} = \mathbf{F}\Phi\mathbf{F}' + \Theta^2 + \mathbf{W}\mathbf{W}' \tag{1}$$

- $\mathbf{P}$: $p \times p$ population correlation matrix
- $\mathbf{F}$: $p \times m$ factor loading matrix
- Φ: $m \times m$ factor correlation matrix
- Θ^2: $p \times p$ matrix of unique item variances
- $\mathbf{W}$: $p \times q$ minor factor loading matrix for the $q \gg m$ minor common factors

Methods

Simulation Conditions

- Major common factors: $m \in \{1, 3, 5, 10\}$
- Items per factor: $p/m \in \{5, 10\}$
- Subjects per item: $N/p \in \{5, 10, 15\}$
- Factor Loading: Loading $\in \{0.4, 0.6, 0.8\}$
- Model Error: $\upsilon_E \in \{0.0, 0.1, 0.3\}$
    - Proportion of uniqueness variance apportioned to minor common factors

Fully-crossed design with 216 unique conditions

Simulation Procedure

For each of the 216 unique conditions, conduct 1,000 replications of the following steps:

1. Generate binary response data using Equation (1)
2. Compute the tetrachoric correlation matrix
3. If the matrix is PSD, next; Else, smooth using:
    - Higham (2002)
    - Bentler-Yuan (2011)
    - Knol-Berger (1991)
4. For each of the three smoothed correlation matrices and the unsmoothed matrix, estimate factor loadings using:
    - Principal Axes factor extraction (PA)
    - Ordinary Least Squares (OLS)
    - Maximum Likelihood (ML)

Given two $p \times p$ symmetric matrices, $\mathbf{A} = \{a_{ij}\}$ and $\mathbf{B} = \{b_{ij}\}$,

$$\mathrm{D_s}(\mathbf{A}, \mathbf{B}) = \sqrt{\sum_{i=1}^{p-1} \sum_{j=i+1}^{p} \frac{\left(a_{ij} - b_{ij}\right)^2}{p(p-1)/2}}.$$

- $\mathbf{R}_{\mathrm{Sm}} \in \{\mathbf{R}_{-}, \mathbf{R}_{\mathrm{APA}}, \mathbf{R}_{\mathrm{BY}}, \mathbf{R}_{\mathrm{KB}}\}$
- $\mathbf{R}_{\mathrm{Pop}} = \mathbf{F}\Phi\mathbf{F}' + \Theta^2 + \mathbf{W}\mathbf{W}'$

Evaluate recovery of $\mathbf{R}_{\mathrm{Pop}}$ using $\mathrm{D_s}(\mathbf{R}_{\mathrm{Sm}}, \mathbf{R}_{\mathrm{Pop}})$

$\mathbf{F}$ Recovery Criterion

Evaluate how well the factor loading matrix, $\mathbf{F}$, was recovered using:

$$\mathrm{RMSE}(\mathbf{F}, \hat{\mathbf{F}}) = \sqrt{\sum_{i=1}^{p} \sum_{j=1}^{m} \frac{\left(f_{ij} - \hat{f}_{ij}\right)^2}{pm}}$$

Results

Indefinite Matrix Frequency

124,346 (57.6%) of 216,000 tetrachoric correlation matrices were indefinite

Indefinite matrices were most common in conditions with:

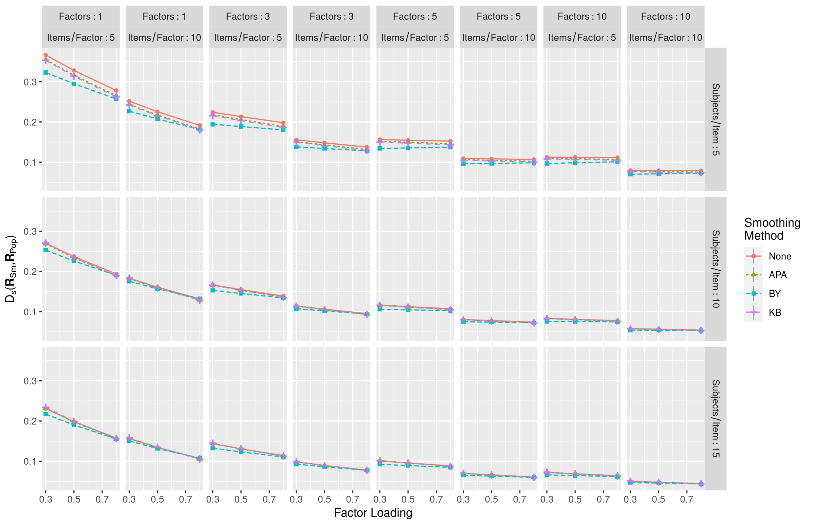
- Many factors/items per factor (i.e., total number of items)
- Few subjects per item
- Large factor loadings

Indefinite Matrix Frequency

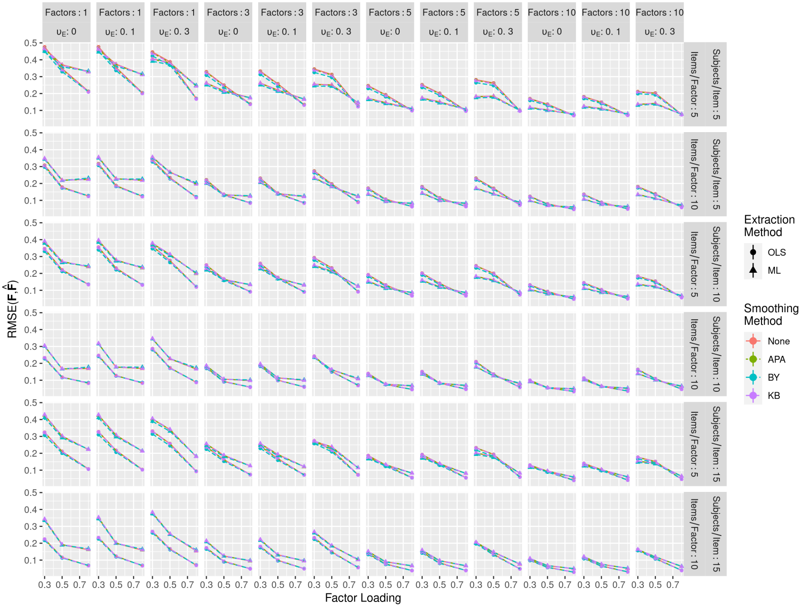
		Factors			
N/p	Loading	1	3	5	10
5	0.3	46.2	98.9	100.0	100.0
5	0.5	52.8	99.7	100.0	100.0
5	0.8	56.4	100.0	100.0	100.0
10	0.3	8.1	22.9	33.0	43.4
10	0.5	16.5	47.7	66.1	85.7
10	0.8	49.1	99.3	100.0	100.0
15	0.3	1.0	0.6	0.4	0.5
15	0.5	2.6	3.7	6.4	16.2
15	0.8	32.8	86.0	96.4	100.0

Note: Percent of indefinite matrices conditioned on number of subjects per item (N/p), factor loading, and number of factors.

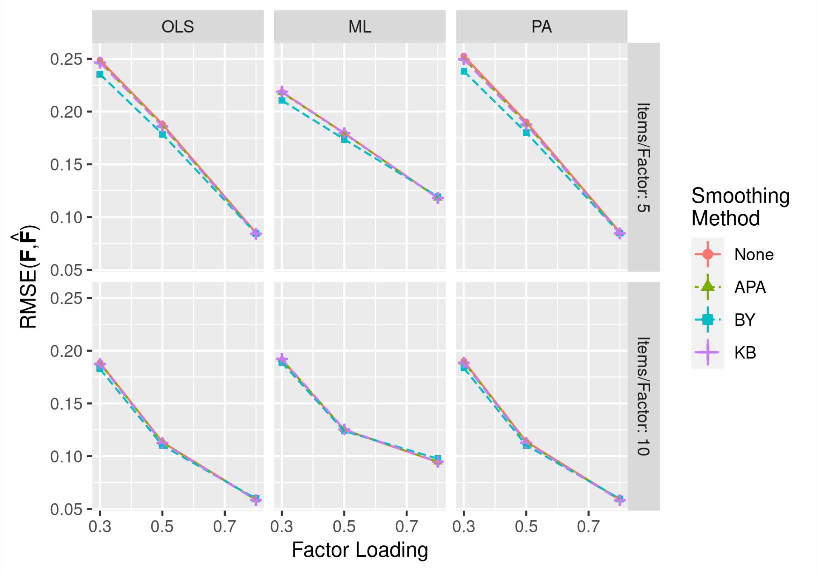
Population Correlation Matrix ($\mathbf{R}_{\mathbf{Pop}}$) Recovery



Factor Loading Recovery



Factor Loading Recovery



Discussion

Summary: Population Correlation Matrix ($\mathbf{R_{Pop}}$) Recovery

- $\mathbf{R}_{\text{Pop}}$ recovery was better in conditions with:
  - High factor loadings
  - Many major factors
  - Many items per factor
  - Many subjects per item
- The Bentler-Yuan (2011) algorithm led to slightly better recovery in conditions with:
  - Low factor loadings
  - Few major factors
  - Few items per factor
  - Few subjects per item

Summary: Factor Loading Recovery

- Factor loading recovery was better in conditions with:
    - High factor loadings
    - Many major factors
    - Many items per factor
    - Small amounts of model approximation error
    - Under these conditions, OLS and PA led to better results than ML
- Bentler-Yuan (2011) led to slightly better results in conditions with:
    - Low factor loadings
    - Few items per factor
    - ML factor extraction

Limitations & Future Directions

- Only orthogonal models with fixed factor loadings
- Investigated only indefinite tetrachoric correlation matrices
    - Polychoric correlation matrices
    - Composite correlation matrices
    - Correlation matrices calculated from missing data
- Investigate methods that avoid the problem
    - Remove problematic items
    - Full-information factor analysis
    - Bayesian/penalized tetrachoric estimation

Simulation Code

https://github.umn.edu/krach018/masters_thesis

Backup Slides

Algorithm 1: For an indefinite correlation matrix $\mathbf{R}\_$, find the nearest PSD correlation matrix

Initialize $\mathbf{S}_0 = 0$; $\mathbf{Y}_0 = \mathbf{R}\_$

for $k = 1, 2, \ldots$ **do**

$\quad \mathbf{Z}_k = \mathbf{Y}_{k-1} - \mathbf{S}_{k-1}$

$\quad \mathbf{X}_k = P_S(\mathbf{Z}_k)$

$\quad \mathbf{S}_k = \mathbf{X}_k - \mathbf{Z}_k$

$\quad \mathbf{Y}_k = P_U(\mathbf{X}_k)$

end

The algorithm continues until convergence occurs or the maximum number of iterations is exceeded. If the algorithm converges, $\mathbf{R}_{\mathrm{APA}} = \mathbf{Y}_k$.

Given a population covariance (correlation) matrix, Σ, minimum trace factor analysis seeks to find the diagonal matrix of unique variances, $\Psi = \mathrm{diag}(\Psi_{11}, \ldots, \Psi_{pp})$ to solve the optimization problem:

$$\underset{\Psi}{\mathrm{Min}}\, \mathrm{tr}(\Sigma - \Psi) \text{ subject to } \Sigma - \Psi \succeq 0 \tag{2}$$

The greatest lower bound of reliability is then defined as:

$$\rho := 1 - \frac{\mathrm{tr}\,\bar{\Psi}}{1_p' \Sigma 1_p}$$

where $\bar{\Psi} = \bar{\Psi}(\Sigma)$ is the optimal solution of Equation (3) (Shapiro & Berge, 2002).

$$\mathbf{H}_0 = \operatorname{diag}(h_1, \ldots, h_p)$$

- h_i is the estimated communality for Item i

Algorithm 2: Extract principal axes factor solution

Initialize $\mathbf{R}_0^* = \mathbf{R} - \mathbf{I} + \mathbf{H}_0$

for $k = 1, 2, \ldots$ **do**

$$\mathbf{R}_{k-1}^* = \mathbf{V}_{k-1}\Lambda_{k-1}\mathbf{V}_{k-1}'$$

$$\mathbf{R}_k^* = \mathbf{R}_{k-1}^* - \mathbf{I} + \Lambda_{k-1}$$

$$\epsilon = |\operatorname{diag}\Lambda_k - \operatorname{diag}\Lambda_{k-1}|$$

end

Stop when $\epsilon \leq \delta$.

Ordinary Least Squares Factor Extraction

$\hat{\mathbf{P}}$: Implied correlation matrix from the estimated factor model

$\mathbf{R}$: Observed correlation matrix

Minimize the discrepancy function:

$$F_{OLS}(\mathbf{R}, \hat{\mathbf{P}}) = \frac{1}{2}\,\mathrm{tr}\left[(\mathbf{R} - \hat{\mathbf{P}})^2\right]$$

Minimize the discrepancy function:

$$F_{ML}(\mathbf{R}, \hat{\mathbf{P}}) = \log|\hat{\mathbf{P}}| - \log|\mathbf{R}| + \mathrm{tr}\left(\mathbf{S}\hat{\mathbf{P}}^{-1}\right) - p$$

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