Simultaneous Inference for Latent Variables in Factor Analytic Models

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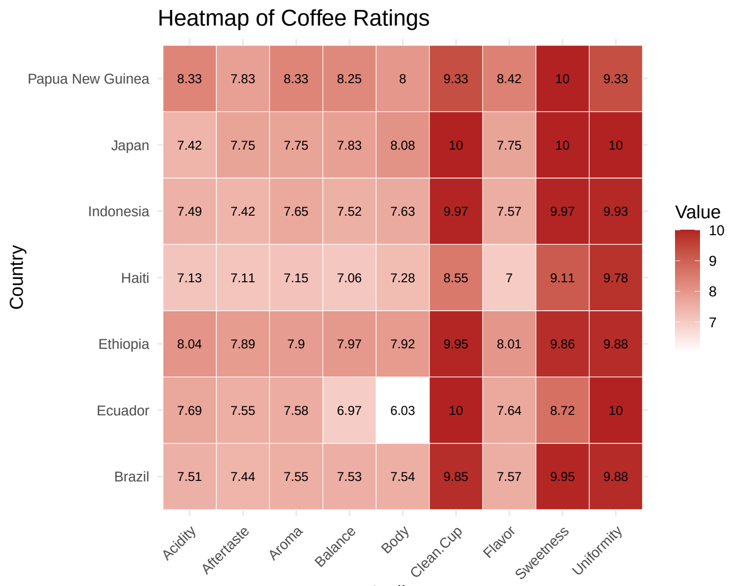
Motivating Data: Coffee Bean Exploration

- The coffee bean dataset records consumer ratings (0–10) on nine sensory attributes (e.g., sweetness, aroma, acidity) and aggregates them by country. The dataset consists of $n = 32$ countries in total.
  - Data are publicly available from Kaggle `https://www.kaggle.com/datasets/adampq/coffee-quality-with-locations-of-origin?resource=download`, which itself is sourced from the Coffee Quality Instiute (CQI) database `https://database.coffeeinstitute.org/`

Motivating Data: Coffee Bean Exploration



Motivating Data: Coffee Bean Exploration

- We hypothesise a few latent factors can be used to represent these observed ratings e.g., latent axis representing aspects of coffee taste or richness. That is, we wish to perform dimension reduction.
- Our interest is to perform statistical inference in this latent space e.g., do two countries differ statistically in terms of coffee taste/richness? Is the ”best” country statistically different from the rest?

The Factor Analytic Model

Suppose we have n independent observations $\mathbf{y}_i; i = 1, 2, \ldots, n$, each of dimension p. Assume the j-th response y_{ij} can be written as (West et al., 2003)

$$y_{ij} = \mathbf{x}_i^\top \boldsymbol{\beta}_j + \mathbf{f}_i^\top \boldsymbol{\lambda}_j + \epsilon_{ij},$$

where

- $\mathbf{x}_i$ is a q-dimensional covariate and $\boldsymbol{\beta}_j$ the associated coefficients;
- $\mathbf{f}_i$ is an m-dimensional latent factor assumed to be standard normal in distribution, $f_{ik} \sim \mathcal{N}(0, 1)$;
- $\boldsymbol{\lambda}_j$ is an m-dimensional loading vector. Furthermore, we define the **loading matrix** $\boldsymbol{\Lambda} = [\boldsymbol{\lambda}_1 \; \boldsymbol{\lambda}_2 \; \cdots \; \boldsymbol{\lambda}_p]^\top$;
- ϵ_{ij} is an error term where we assume $\epsilon_{ij} \sim \mathcal{N}(0, \psi_{jj})$.

- We write the fully vectorised form of the factor analytic model as,

$$\boldsymbol{y} = (\mathbf{I}_p \otimes \mathbf{X})\, \boldsymbol{\beta} + (\boldsymbol{\Lambda} \otimes \mathbf{I}_n)\, \boldsymbol{f} + \boldsymbol{\epsilon},$$

  where $\boldsymbol{y} = (y_{11}, \cdots, y_{n1}, y_{12}, \cdots, y_{np})^\top$, $\mathbf{X}^\top = \left[\mathbf{x}_1^\top\ \mathbf{x}_2^\top\ \ \ldots\ \mathbf{x}_n^\top\right]$ is an $q \times n$ matrix, $\boldsymbol{\beta} = \left(\boldsymbol{\beta}_1^\top, \boldsymbol{\beta}_2^\top, \boldsymbol{\beta}_p^\top\right)^\top$, $\boldsymbol{f} = (f_{11}, \cdots, f_{n1}, f_{12}, \cdots, f_{np})^\top$ and $\boldsymbol{\epsilon} = (\epsilon_{11}, \cdots, \epsilon_{n1}, \epsilon_{12}, \cdots, \epsilon_{np})^\top$.
- Marginally, we have

$$\boldsymbol{y} \sim \mathcal{N}_{np}\left((\mathbf{I}_p \otimes \mathbf{X})\, \boldsymbol{\beta}, \mathbf{V} \otimes \mathbf{I}_n\right),$$

  where $\mathbf{V} = \boldsymbol{\Lambda}\boldsymbol{\Lambda}^\top + \boldsymbol{\Psi}$ is the marginal variance of each observation $\mathbf{y}_i$, and we call $\boldsymbol{\theta} := \left[\mathrm{vec}(\boldsymbol{\Lambda})^\top, \mathrm{diag}(\boldsymbol{\Psi})^\top\right]^\top$ the **variance components**.

Model Identifiability

- Without any constraints on the loading matrix $\mathbf{\Lambda}$, the factor model is not identifiable, since for any orthogonal matrix $\mathbf{M}$, the transformed loading matrix $\mathbf{\Lambda M}$ yields the same covariance structure and the same likelihood (Mardia et al., 1979).
- We put a **corner constraint** on the loading matrix by setting the upper-triangular elements of $\mathbf{\Lambda}$ to zero, and restrict the diagonal elements of $\mathbf{\Lambda}$ to be positive.

Parameter Estimation and Factor Prediction

Given variance component $\boldsymbol{\theta}$,

- the MLE of $\boldsymbol{\beta}$ is
$$\hat{\boldsymbol{\beta}} = \left(\mathbf{I}_p \otimes (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top\right) \boldsymbol{y},$$
- the best linear unbiased prediction (BLUP) (Searle et al., 2009) of $\boldsymbol{f}$ is
$$\tilde{\boldsymbol{f}} = \mathbb{E}\left[\boldsymbol{f} \mid \boldsymbol{y}\right] = \left(\boldsymbol{\Lambda}^\top \mathbf{V}^{-1} \otimes \mathbf{I}_n\right)\left(\boldsymbol{y} - (\mathbf{I}_p \otimes \mathbf{X})\hat{\boldsymbol{\beta}}\right).$$

In practice, we can plug in estimated values of $\hat{\boldsymbol{\theta}}$ (e.g. obtained via REML (Corbeil and Searle, 1976)) to obtain $\hat{\boldsymbol{f}}$.

General Mixed Parameters

We are interested in conduct simultaneous inference for a set of L general mixed parameters. For known designed vectors $\boldsymbol{c}_l$ and $\boldsymbol{\kappa}_l$, the **general mixed parameter** (Reluga et al., 2023) for level $l = 1, \ldots, L$ is given by

$$\mu_l = \boldsymbol{c}_l^\top \boldsymbol{\beta} + \boldsymbol{\kappa}_l^\top \boldsymbol{f}$$

The BLUP for the general mixed parameter is then given by plugging $\hat{\boldsymbol{\beta}}$ and $\tilde{\boldsymbol{f}}$,

$$\tilde{\mu}_l = \boldsymbol{c}_l^\top \hat{\boldsymbol{\beta}} + \kappa_l^\top \tilde{\boldsymbol{f}},$$

and the empirical BLUP or EBLUP follows us

$$\hat{\mu}_l = \boldsymbol{c}_l^\top \hat{\boldsymbol{\beta}} + \kappa_l^\top \hat{\boldsymbol{f}}.$$

Prediction Mean Square Error

- For level $l = 1, \ldots, L$, the **prediction mean square error** (PMSE) $\sigma^2(\hat{\mu}_l)$ can be decomposed as

$$\begin{aligned}\mathbb{E}[(\hat{\mu}_l - \mu_l)^2] &= \mathbb{E}[(\hat{\mu}_l - \tilde{\mu}_l)^2] + \mathbb{E}[(\tilde{\mu}_l - \mu_l)^2] + 2\mathbb{E}[(\hat{\mu}_l - \tilde{\mu}_l)(\tilde{\mu}_l - \mu_l)] \\ &= \mathbb{E}[(\hat{\mu}_l - \tilde{\mu}_l)^2] + \sigma^2(\tilde{\mu}_l).\end{aligned}$$

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- As $n \to \infty$ the second term dominates the PMSE of $\hat{\mu}_l$, where

$$\sigma^2(\tilde{\mu}_l) = \boldsymbol{\kappa}_l^\top \boldsymbol{\kappa}_l - \boldsymbol{\kappa}_l^\top ((\boldsymbol{\Lambda}^\top \mathbf{V}^{-1} \boldsymbol{\Lambda}) \otimes \mathbf{I}_n) \boldsymbol{\kappa}_l + (\boldsymbol{c}_l - (\mathbf{I}_p \otimes \mathbf{X}^\top) \boldsymbol{o}_l)^\top \mathbf{Q} (\boldsymbol{c}_l - (\mathbf{I}_p \otimes \mathbf{X}^\top) \boldsymbol{o}_l)$$

  where $\boldsymbol{o}_l = (\mathbf{V}^{-1} \boldsymbol{\Lambda} \otimes \mathbf{I}_n) \boldsymbol{\kappa}_l$ and $\mathbf{Q} = \mathbf{V} \otimes (\mathbf{X}^\top \mathbf{X})^{-1}$.
- We approximate $\hat{\sigma}^2(\hat{\mu}_l) \approx \hat{\sigma}^2(\tilde{\mu}_l)$, based on by plugging the estimated variance components.

Basic Idea: CPI vs. SPI

- A cluster-level prediction interval (CPI) is an region $\mathcal{C}_{1-\alpha}$ such that it has probability $100(1-\alpha)\%$ of covering the general mixed parameter **for a single level**.

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- A simultaneous prediction interval (SPI) is a region $\mathcal{I}_{1-\alpha}$ such that it has probability $100(1-\alpha)\%$ of covering the general mixed parameters **across all levels**,

$$\mathbb{P}(\mu_l \in \mathcal{I}_{1-\alpha}, \forall l \in [L]) = 1-\alpha.$$

Constructing SPIs

- From the equation $\mathbb{P}(\mu_l \in \mathcal{I}_{1-\alpha}, \forall l \in [L]) = 1-\alpha$ suggests a maximum t-type statistic:

$$\begin{aligned}\alpha &= \mathbb{P}(\mu_l \notin \mathcal{I}_{1-\alpha}, \exists l \in [L]) \\ &= \mathbb{P}\left(\left|\frac{\hat{\mu}_l - \mu_l}{\hat{\sigma}(\hat{\mu}_l)}\right| \geqslant c_{1-\alpha}, \exists l \in [L])\right) \\ &= \mathbb{P}\left(\max_{l=1,2,\ldots,L}\left|\frac{\hat{\mu}_l - \mu_l}{\hat{\sigma}(\hat{\mu}_l)}\right| \geqslant c_{1-\alpha}\right).\end{aligned}$$

- Theoretically, the critical value $c_{1-\alpha}$ is then the $(1-\alpha)^{\text{th}}$-quantile of the maximum t-type statistic i.e.,

$$c_{1-\alpha} = \inf_t \{t \in \mathbb{R} : \mathbb{P}(\tau \leqslant t) \geqslant 1-\alpha\},$$

where $\tau = \max_{l=1,2,\ldots,L} |\tau_l|$ and $\tau_l = \frac{\hat{\mu}_l - \mu_l}{\hat{\sigma}(\hat{\mu}_l)}$.

- If $c_{1-\alpha}$ is known, the SPI can be constructed as

$$\mathcal{I}_{1-\alpha} = \bigtimes_{l=1}^{L} \left[\hat{\mu}_l \mp c_{1-\alpha}\hat{\sigma}(\hat{\mu}_l)\right].$$

Approximate the Critical Value $c_{1-\alpha}$

We propose three ways to approximate the $c_{1-\alpha}$: the **Bootstrap method**, the **Monte Carlo method**, and the **Bonferroni method**. In this talk, we will focus on the bootstrap method.

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3. For each bootstrap dataset, fit the model again to **obtain the bootstrap version of the maximum t-type statistics**.
4. Use the $1 - \alpha$ quantile of the bootstrap empirical distribution of the maximum t-type statistics $c_{1-\alpha}^{BS}$.

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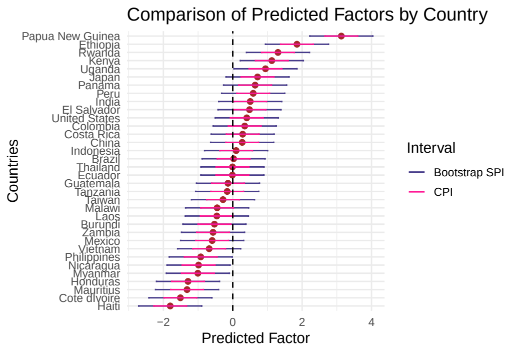
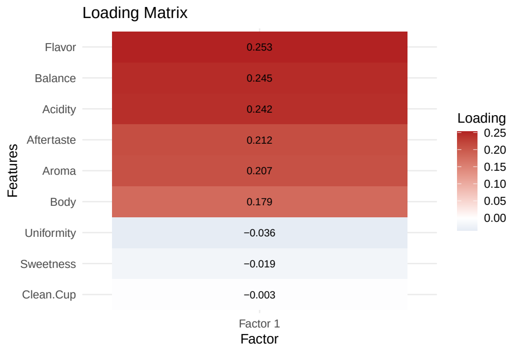
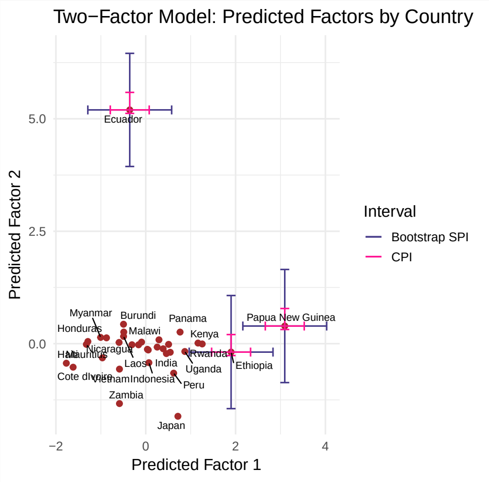
3. For each bootstrap dataset, fit the model again to **obtain the bootstrap version of the maximum t-type statistics**.
4. Use the $1-\alpha$ quantile of the bootstrap empirical distribution of the maximum t-type statistics $c_{1-\alpha}^{BS}$.
5. **Construct SPI** using $c_{1-\alpha}^{BS}$ and the results from Step 1, $\mathcal{I}_{1-\alpha}^{BS} = \times_{l=1}^{L} \left[\hat{\mu}_l \mp c_{1-\alpha}^{BS} \hat{\sigma}(\hat{\mu}_l)\right]$.

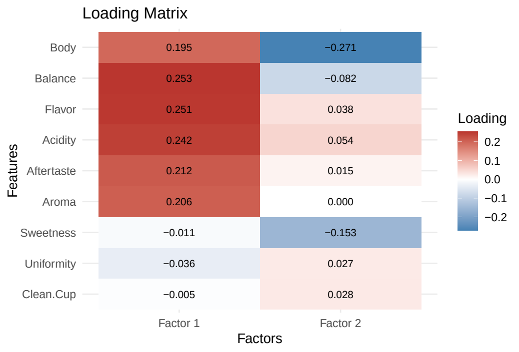
Application to Coffee Bean Data: 1-factor Model





Application to Coffee Bean Data: 2-factor Model





Discussion

- Simultaneous inference can be useful in the context of factor analytic models, if we want to perform (say) formal statistical inference on the latent variables.
- We proposed constructing SPI using a bootstrap approach. In simulations (not shown), we show **this generically performs better than** simpler Monte Carlo- and Bonferroni-based SPIs.
- In future work, we will run more simulations under more complicated models and general mixed parameters, as well as investigate simultaneous inference the case of non-Gaussian response factor analytic models.

Thank You!

Let's drink a cup of coffee and see whether my research aligns with your tastes!

Questions?

References

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Appendix

Using the mixed model equation, we find

$$\begin{bmatrix} \tilde{\boldsymbol{\beta}} - \boldsymbol{\beta} \\ \tilde{\boldsymbol{f}} - \boldsymbol{f} \end{bmatrix} \sim \mathcal{N}_{qp+nm}\left(\mathbf{0}_{qp+nm}, \left(\hat{\mathbf{A}}^\top \hat{\mathbf{K}}^{-1} \hat{\mathbf{A}} + \hat{\mathbf{B}}\right)^{-1}\right),$$

where $\hat{\mathbf{A}} := \begin{bmatrix} \mathbf{I}_p \otimes \mathbf{X} & \hat{\boldsymbol{\Lambda}} \otimes \mathbf{I}_n \end{bmatrix}$, $\hat{\mathbf{B}} := \begin{bmatrix} \mathbf{0}_{qp \times qp} & \mathbf{0}_{qp \times nm} \\ \mathbf{0}_{nm \times qp} & \mathbf{I}_{nm} \end{bmatrix}$, and $\hat{\mathbf{K}} := \hat{\boldsymbol{\Psi}} \otimes \mathbf{I}_n$.

Therefore for a Monte Carlo Procedure, for $s = 1, 2, \ldots, S$:

1. Sample $\begin{bmatrix} \tilde{\boldsymbol{\beta}} - \boldsymbol{\beta} \\ \tilde{\boldsymbol{f}} - \boldsymbol{f} \end{bmatrix}^{(s)}$ from its asymptotic distribution.
2. Calculate the centred general mixed effect $(\mu_l - \mu)^{(s)} = \boldsymbol{c}_l^\top (\tilde{\boldsymbol{\beta}} - \boldsymbol{\beta})^{(s)} + \boldsymbol{\kappa}_l^\top (\tilde{\boldsymbol{f}} - \boldsymbol{f})^{(s)}$.
3. Calculate $\tau_{MC}^{(s)} := \max_l \frac{|(\mu_l - \mu)^{(s)}|}{\hat{\sigma}(\hat{\mu}_l)}$.

Order $\tau_{MC}^{(s)}$ for all $s \in [S]$ and find the upper $1 - \alpha$ quantile as the empirical critical value $c_{1-\alpha}^{\mathsf{MC}}$.

Bonferroni Procedure

In a Bonferroni procedure, we directly approximate the critical value as $c^{\mathsf{BO}}_{1-\alpha} = \Phi^{-1}\left(1 - \frac{\alpha}{2L}\right)$, where $\Phi^{-1}(\cdot)$ is the quantile function of the standard normal distribution.

Simulation Settings

- It is of interest to see how SPIs constructed by different methods behave under different n, p, q, m, along with the true variance explained (VE) by the loadings

$$\mathrm{VE} = \frac{\mathrm{tr}(\boldsymbol{\Lambda}\boldsymbol{\Lambda}^\top)}{\mathrm{tr}(\boldsymbol{\Lambda}\boldsymbol{\Lambda}^\top + \boldsymbol{\Psi})}.$$

- We ran 200 simulation rounds for different combinations of $(n, p, q, m, \mathrm{VE})$.
- The **target** of the intervals was all the latent variables in a one-factor model i.e., $L = n$.
- We used $B = 500$ bootstrap datasets and $S = 2000$ Monte Carlo samples.

Simulation Results

Table 1: Summary of SPI methods across different simulation settings ($p = 20$, $m = 1$, $q = 3$). The nominal level of intervals is 0.95.

Setting	Method (Intervals)	ECP	Mean Len.	Avg Var-Width ($\times 10^{-2}$)
$n = 500$, VE$= 0.7$	Bootstrap SPI	0.949	1.30	0.13
	Monte Carlo SPI	0.913	1.26	0.11
	Bonferroni SPI	0.924	1.27	0.10
	CPI	0	0.57	0.03
$n = 200$, VE$= 0.7$	Bootstrap SPI	0.965	1.43	0.27
	Monte Carlo SPI	0.915	1.35	0.22
	Bonferroni SPI	0.930	1.37	0.19
	CPI	0	0.57	0.09
$n = 500$, VE$= 0.5$	Bootstrap SPI	0.940	1.82	0.31
	Monte Carlo SPI	0.935	1.78	0.25
	Bonferroni SPI	0.935	1.79	0.25
	CPI	0	0.85	0.07

Takeaways from Simulations

- **Bootstrap SPI performs well**, achieving empirical coverage closest to the nominal 0.95 level.
- **As sample size increases**, Monte Carlo and Bonferroni SPIs are still slightly undercovered.
- **Lower VE increases uncertainty**, resulting in longer interval lengths and larger average variance of interval widths.
- **CPI consistently fails to provide valid coverage**, highlighting the necessity of simultaneous inference.