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To cite this version:

Francesco Amato, Julien Jacques. Clustering Longitudinal Ordinal Data. StatLearn, Apr 2022, Cargèse, France. hal-03657085

HAL Id: hal-03657085

https://hal.univ-lyon2.fr/hal-03657085

Submitted on 2 May 2022

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Clustering Longitudinal Ordinal Data

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Context

- Longitudinal ordinal data $y_{i,j,t}$ whose levels are coded $\{1, \dots, C_j\}$: the observation of the j-th variable for the i-th unit at time t $(i = 1, \dots, N; j = 1, \dots, J$ and $t = 1, ..., T)$.
- We want to **cluster units accounting for the temporal behavior**
- $\Rightarrow$ 💡 Idea: rewrite them in a three-way format and use **latent underlying continous matrix-variate distributions**!
- We organize our data in a random-matrix form such that:

$$Y_i = \begin{pmatrix} y_{i,1,1} & \cdots & y_{i,1,t} & \cdots & y_{i,1,T} \\ \vdots & \ddots & \vdots & \cdots & \vdots \\ y_{i,j,1} & \cdots & y_{i,j,t} & \cdots & y_{i,j,T} \\ \vdots & \cdots & \vdots & \ddots & \vdots \\ y_{i,J,1} & \cdots & y_{i,J,t} & \cdots & y_{i,J,T} \end{pmatrix}$$

From continuous...

- Matrix-variate Normal: $Z \sim \mathcal{MN}_{(J\times T)}(M, \Phi, \Sigma)$, where
  - $M \in \mathbb{R}^{J\times T}$ is the matrix of means
  - $\Phi \in \mathbb{R}^{T\times T}$ is a covariance matrix between the T occasions
  - $\Sigma \in \mathbb{R}^{J\times J}$ is the covariance matrix of the J variables

  The matrix-normal probability density function (pdf) is given by

$$\phi^{(J\times T)}(Z|M, \Phi, \Sigma) =$$
$$(2\pi)^{-\frac{TJ}{2}}|\Phi|^{-\frac{J}{2}}|\Sigma|^{-\frac{T}{2}} \exp\left\{-\frac{1}{2}\mathrm{tr}[\Sigma^{-1}(Z - M)\Phi^{-1}(Z - M)^\intercal]\right\}$$

- Mixtures of Matrix-Normals (MMN) were introduced by Viroli [3]

$$f(Y|\boldsymbol{\pi}, \boldsymbol{\Theta}) = \sum_{k=1}^{K} \pi_k \phi^{(J\times T)}(Z|M_k, \Phi_k, \Sigma_k),$$

  where
  - K : number of mixture components
  - $\boldsymbol{\pi} = \{\pi_k\}_{k=1}^K$: vector of mixing proportions, $\sum_{k=1}^K \pi_k = 1$
  - $\boldsymbol{\Theta} = \{\Theta_k\}_{k=1}^K$: set of component-specific parameters $\Theta_k = \{M_k, \Phi_k, \Sigma_k\}$

$\Longrightarrow$ **Advantages**: offers a parsimonious and easily interpretable way to include the time dimension in the clustering.

...to ordinal data!

In the `clustMD` framework [2] cross-sectional mixed data are assumed to be all manifestation of underlying multivariate normals, and a Gaussian mixture model operating on the underlying normal variable is used to cluster them.

As for the classical `clustMD`, we can assume that each observed ordinal matrix Y is indeed the manifestation of a latent random matrix Z, which follows a matrix-normal distribution.

$$Z_i = \begin{pmatrix} z_{i,1,1} & \cdots & z_{i,1,t} & \cdots & z_{i,1,T} \\ \vdots & \ddots & \vdots & \cdots & \vdots \\ z_{i,j,1} & \cdots & z_{i,j,t} & \cdots & z_{i,j,T} \\ \vdots & \cdots & \vdots & \ddots & \vdots \\ z_{i,J,1} & \cdots & z_{i,J,t} & \cdots & z_{i,J,T} \end{pmatrix} \longrightarrow Y_i = \begin{pmatrix} y_{i,1,1} & \cdots & y_{i,1,t} & \cdots & y_{i,1,T} \\ \vdots & \ddots & \vdots & \cdots & \vdots \\ y_{i,j,1} & \cdots & y_{i,j,t} & \cdots & y_{i,j,T} \\ \vdots & \cdots & \vdots & \ddots & \vdots \\ y_{i,J,1} & \cdots & y_{i,J,t} & \cdots & y_{i,J,T} \end{pmatrix}$$

To map from Y_i to Z_i, let γ_j denote a C_j+1-dimensional vector of thresholds that partition the space of the underlying latent continuous variable for the j-th ordinal variable. Let the threshold parameters be constrained such that $-\infty = \gamma_{j,0} \leq \gamma_{j,1} \leq ... \leq \gamma_{j,C_j} = \infty$. If the latent $z_{i,j,t}$ is such that $\gamma_{j,c-1} < z_{i,j,t} < \gamma_{j,c}$ then the observed ordinal response, $y_{i,j,t} = c$.

A key point is of course the choice of the thresholds $\boldsymbol{\gamma} = \{\gamma_j\}_{j=1}^J$. In [1], thresholds are fixed in advance to avoid identifiability and computational complexity issues. Also in [2], for ordinal variables they are fixed such that $\gamma_{j,c} = \varphi^{-1}(\delta_c)$, where δ_c is the proportion of variable J which are less than or equal to level c and φ is the normal cumulative distribution function.

Model

The model relies on the following hypotheses:

- $\boldsymbol{\ell}_i \in \{0, 1\}^K$ is the latent allocation variable such that $\ell_{ik} = 1$ if the i-th unit belongs to the k-th cluster.
- $\mathbf{Y}_i^R = (Y_{i1}^R, ..., Y_{iR}^R) \in \mathbb{R}^R$ indicate the observed response pattern for the i-th unit.
- $\boldsymbol{\ell}_i \sim \mathcal{M}(1, \boldsymbol{\pi})$, $\boldsymbol{\pi} = (\pi_1, ..., \pi_K)$
- $\mathbf{Z}_i|\boldsymbol{\ell}_{ik} = 1 \sim \mathcal{MN}_{(J\times T)}(\mathbf{Z}_i|\Theta_k)$, $\Theta_k = \{M_k, \Phi_k, \Sigma_k\}$
- $\mathbf{Y}_i^R|\mathbf{Z}_i, \boldsymbol{\ell}_{ik} = 1 \sim \mathcal{M}(1, \boldsymbol{\xi}_i^R)$, $\boldsymbol{\xi}_i^R = (\mathbf{1}_{\Omega_1}(\mathbf{Z}_i), \dots, \mathbf{1}_{\Omega_R}(\mathbf{Z}_i))$

where $\mathcal{M}$ indicate the multinomial distribution, Ω_r is the portion of the $J \times T$-space which determines the the r-th pattern, and $\mathbf{1}_{\Omega_r}(\mathbf{Z}_i)$ is the indicator function that equals 1 when the elements in $\mathbf{Z}_i$ have values that determine the r-th pattern. Of course, when $\mathbf{Z}_i$ is given, the the value of $\mathbf{Y}_i$ is no more random.

We can derive the joint density of $\mathbf{Z}_i, \mathbf{Y}_i^R, \boldsymbol{\ell}_i$ as:

$$f(\mathbf{Y}_i^R, \mathbf{Z}_i, \boldsymbol{\ell}_i) = f(\mathbf{Y}_i^R|\mathbf{Z}_i, \boldsymbol{\ell}_i) f(\mathbf{Z}_i|\boldsymbol{\ell}_i) f(\boldsymbol{\ell}_i),$$

where:

$$f(\boldsymbol{\ell}_i) = \prod_{k=1}^{K} \pi_k^{\ell_{ik}}, f(\mathbf{Z}_i|\boldsymbol{\ell}_i) = \prod_{k=1}^{K} \left[\phi^{(J\times T)}(Z_i|\Theta_k)\right]^{\ell_{ik}}, f(\mathbf{Y}_i^R|\mathbf{Z}_i, \boldsymbol{\ell}_i) = \prod_{r=1}^{R} \mathbf{1}_{\Omega_r}(Z_i)^{Y_{ir}^R}$$

Model Inference

Due to the presence of latent variables, the maximization of the likelihood cannot be done in "close form", and we must then use an EM algorithm, which maximizes a lower limit of the log-likelihood: the complete log-likelihood. We can write the complete log-likelihood as

$$\log \mathcal{L}_{\mathcal{C}}(\boldsymbol{\pi}, \boldsymbol{\Theta}|\mathbf{Y}^R, \mathbf{Z}, \boldsymbol{\ell}) = \sum_{i=1}^{N}\left\{\sum_{r=1}^{R} Y_{ir}\mathbf{1}_{\Omega_r}(Z_i) + \sum_{k=1}^{K} \ell_{ik}\left[\log(\pi_k) - \frac{TJ}{2}\log(2\pi)\right.\right.$$
$$\left.\left. - \frac{J}{2}\log(|\Phi_k|) - \frac{T}{2}\log(|\Sigma_k|) - \frac{1}{2}tr[\Sigma_k^{-1}(Z_i - M_k)\Phi_k^{-1}(Z_i - M_k)^\intercal]\right]\right\}.$$

- E-step: we compute the expectation of the complete log-likelihood with respect to the latent data Z and the cluster labels ℓ. For each response pattern r, **we can approximate the value of $\mathbf{Z}_i|\boldsymbol{\ell}_i$ as the expected value of the truncated multivariate normals (using properties of matrix-variate normals)**, given the parameters Θ_k of the assigned cluster.

  The latent variable $\boldsymbol{\ell}_i$ can be computed by means of Bayes' theorem as:

$$\mathbb{E}(\ell_{ik}^{(s)}|Y_i^R = r, \boldsymbol{\Theta}^{(s-1)}, \boldsymbol{\pi}^{(s-1)}) = \frac{\pi_k^{(s-1)} \int_{\Omega_r} f(Z|\Theta_k^{(s-1)})dZ}{\sum_{k=1}^K \pi_k^{(s-1)} \int_{\Omega_r} f(Z|\Theta_k^{(s-1)})dZ},$$

  which would require Monte-Carlo approximation.

- M-step: the parameter updates are given by:

$$\hat{\Sigma}_k^{(s)} = \frac{\sum_{i=1}^N \ell_{ik}^{(s)}(Z_i - \hat{M}_k^{(s)})\hat{\Phi}_k^{-1(s-1)}(Z_i - \hat{M}_k^{(s)})^\intercal}{T\sum_{i=1}^N \ell_{ik}^{(s)}} \quad , \quad \hat{M}_k^{(s)} = \frac{\sum_{i=1}^N \ell_{ik}^{(s)} Z_i}{\sum_{i=1}^N \ell_{ik}^{(s)}}$$

$$\hat{\Phi}_k^{(s)} = \frac{\sum_{i=1}^N \ell_{ik}^{(s)}(Z_i - \hat{M}_k^{(s)})^\intercal\hat{\Sigma}_k^{-1(s)}(Z_i - \hat{M}_k^{(s)})}{J\sum_{i=1}^N \ell_{ik}^{(s)}} \quad , \quad \hat{\pi}_k^{(s)} = \frac{\sum_{i=1}^N \ell_{ik}^{(s)}}{N}$$

The E and M step are iterated until convergence of the log-likelihood.

A longitudinal `clustMD`? 🧐

This is the first step of a broader project, aiming at extending this framework to account for mixed data (continuous, ordinal, nominal, count) in order to cluster mixed longitudinal dataset.

References

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