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A Few Words on Variable Selection

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Introduction

- We have seen some approaches to dimension reduction, e.g., PCA, factor analysis, the PGMM family, etc.
- McNicholas (2016) refers to dimension reduction as implicit or explicit.
- We have also seen another, and explicit, form of dimension reduction known as variable selection.
- We carried out variable selection when we built (logistic) regression models, e.g., using the step() function, the AICs, or the adjusted \mathbb{R}^2 values.

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Variable Selection

- Consider clustering and classification problems.
- Dimension reduction is important because the presence of variables that are not helpful in discriminating groups can have a deleterious effect on clustering, or classification, performance.
- We have seen the PGMM family, which can be considered an implicit form of dimension reduction.
- There are also variable selection approaches available, which give an explicit dimension reduction.

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VSCC

- The VSCC technique (Andrews and McNicholas, 2014) finds a subset of variables that simultaneously minimizes the within-group variance and maximizes the between-group variance.
- Note that the within-group variance for variable j can be written

$$W_j = \frac{\sum_{g=1}^{G} \sum_{i=1}^{n} z_{ig} (x_{ij} - \mu_{gj})^2}{n}.$$

- The variance within variable j that is not accounted for by \mathcal{W}_j , i.e., $\sigma_j^2 \mathcal{W}_j$, provides an indication of the variance between groups.
- If the data are standardized to have equal variance across variables, then any variable minimizing the within-group variance also maximizes the leftover variance.

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VSCC contd.

 $\bullet\,$ If V represents the space of currently selected variables, then variable j is selected if

$$|\rho_{jr}| < 1 - \mathcal{W}_i^m$$

for all $r \in V$, where $m \in \{1, \dots, 5\}$ is fixed.

- Further details on the VSCC approach are given by Andrews and McNicholas (2014) and McNicholas (2016, Chapter 4).
- The VSCC approach can be used for clustering or semi-supervised classification, and is supported by the vscc package (Andrews and McNicholas, 2013) for R.

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clustvarsel and selvarclust

- Raftery and Dean (2006) propose a variable selection method that utilizes a greedy search of the model space; their approach is based on Bayes factors.
- ullet Given data ${f x}$, the Bayes factor B_{12} for model ${\cal M}_1$ versus model ${\cal M}_2$ is

$$B_{12} = \frac{p(\mathbf{x} \mid \mathcal{M}_1)}{p(\mathbf{x} \mid \mathcal{M}_2)}.$$

where

$$p(\mathbf{x} \mid \mathcal{M}_k) = \int p(\mathbf{x} \mid \boldsymbol{\theta}_k, \mathcal{M}_k) p(\boldsymbol{\theta}_k \mid \mathcal{M}_k) d\boldsymbol{\theta}_k,$$

 θ_k is the vector of parameters for model \mathcal{M}_k , and $p(\theta_k \mid \mathcal{M}_k)$ is the prior distribution of \mathcal{M}_k (Kass and Raftery, 1995).

clustvarsel and selvarclust cont.

- Like VSCC, the approach of Raftery and Dean (2006) simultaneously selects a variable subset, the number of components, and the model, i.e., the GPCM covariance structure.
- The approach of Raftery and Dean (2006) is implemented within the clustvarsel package Dean et al. (2015) for R.
- A related approach, selvarclust, is described by Maugis et al. (2009a,b).

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Comments

- Because the number of free model parameters for some of the GPCM models is quadratic in data dimensionality, clustvarsel, selvarclust, and vscc are largely ineffective in high dimensions.
- In addition to approaches like PGMM, there are other very effective approaches for implicit dimension reduction, e.g., GMMDR (Scrucca, 2010) and HD-GMM (Bouveyron et al., 2007).
- Two good starting places for further reading are Bouveyron and Brunet-Saumard (2014) and McNicholas (2016, Ch. 4).

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