Exploration of the variability of variable selection based on distances between bootstrap sample results

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1 The problem

Regression variable selection can be very unstable. Different models may yield very similar fits; an ambiguous dataset may allow multiple quite different fits.

$$\mathbf{y}_i = \beta_0 + \beta_1 \mathbf{x}_{i1} + \beta_2 \mathbf{x}_{i2} + \ldots + \beta_p \mathbf{x}_{ip} + \mathbf{e}_i,$$

 $i = i, ..., n, e_i \sim \mathcal{N}(0, \sigma^2)$ iid. Variable selection: choose $V \subseteq \{1, ..., p\}$: $j \notin V \Leftrightarrow \beta_j = 0.$

Variable selection can be useful, but it can also be problematic and is easily misinterpreted.

Exploring its stability and a variety of models gives a more comprehensive picture of how the variables "collaborate".

Here: Use LS linear regression, backward selection with AIC or BIC stopping criterion.

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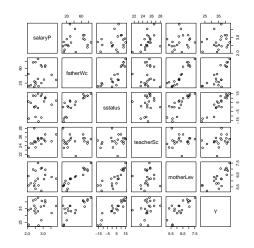
But our techniques are much more general, could use with GLMs, robust regression, Lasso, forward selection, trees and forests...

Dataset 1: (Coleman et al. 1966)

- Data on n = 20 schools,
- y: verbal mean test score,
- x1: staff salary per pupil,
- x₂: percentage of white collar fathers,
- x₃: socioeconomic status composition indicator,
- x₄: mean teacher's verbal test score,
- x_5 : mean mother's educational level.

The problem Ingredients Data analysis

What we learnt



Dataset 2

Study on ozone effects on school childrens lung growth, n = 496 children, p = 24. Ihorst et al. (2004), Buchholz et al. (2008).

Sauerbrei et al. (2015) investigate stability of variable selection using nonparametric bootstrap.

Response: FFVC - forced vital capacity (I) in autumn 1997 Explanatory variables: ALTER age (years) at 1996-03-01 ADHEU allergic rhinitis diagnosed by physician SEX 0male, 1female HOCHOZON patient lives in a village with high ozone values AMATOP maternal atopy (asthma, allergic rhinitis, eczema) AVATOP paternal atopy (asthma, allergic rhinitis, eczema) ADEKZ eczema diagnosed by physician ARAUCH Tobacco smoke exposure at home (no/ves) AGEBGEW weight (g) at birth FSNIGHT cough at night or in the morning FLGROSS height (cm) at pulmonary function testing FMILB sensitization to dust mite allergens FNOH24 maximal NO2 value of last 24h before pulmonary function testing ($\mu q/m3$) FTIER sensitization to animal (dog and cat) danders FPOLL sensitization to pollens (hazel, birch, grass) FLTOTMED total number of medications at pulmonary function testing FO3H24 max. O3 value of last 24h before pulmonary function testing (µg/m3) FSPT sensitization to any of pollens, dog and cat danders or dust mites FTEH24 max. temperature of last 24h before pulmonary function testing (Cel.) ESATEM shortness of breath FSAUGE itchy or watery eyes FLGEW weight (kg) at pulmonary function testing FSPFEI wheezing or whistling in the chest FSHLAUF cough following exercise

Distances Multidimensional Scaling Cluster analysis

2 Ingredients

Analysis uses *B* bootstrap models (selected variables) V_1, \ldots, V_B .

Schools data: B = 500 finds 17 models (backward/AIC). Ozone data: B = 500 each backward/AIC and backward/BIC finds 798 models.

2.1 Distances

Use distance-based methods: Multidimensional scaling, cluster analysis.

Distances Multidimensional Scaling Cluster analysis

Distances between models

(a) Variable-based distance (Kulczynski 1927)

$$d_V(V_1, V_2) = 1 - \left(\frac{|V_1 \cap V_2|}{2|V_1|} + \frac{|V_1 \cap V_2|}{2|V_2|} \right)$$

Can also apply as distance between variables according to presence in models.

Distances Multidimensional Scaling Cluster analysis

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Distances Multidimensional Scaling Cluster analysis

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(b) Fit-based distance

$$d_F(V_1, V_2) = \sum_{i=1}^n |f_{V_1}(\mathbf{x}_i) - f_{V_2}(\mathbf{x}_i)|$$

(Manhattan-distance gives every fit difference same weight.)

Distances Multidimensional Scaling Cluster analysis

2.2 Multidimensional Scaling

Kruskal's (1964) nonmetric MDS maps distances on Euclidean space with distances \hat{d} , optimising

$$\mathsf{Stress} = \sqrt{rac{\sum_{i,j} [f(d(z_i, z_j)) - \hat{d}_{ij}]}{\sum_{i,j} \hat{d}_{ij}}},$$

f monotonic transformation.

Distances Multidimensional Scaling Cluster analysis

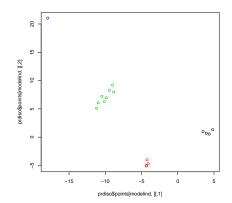
2.3 Suitable clustering methods

E.g., hierarchical (single, complete, average linkage). Use average linkage (AL) here. SL allows large within-cluster distances too easily, CL too often divides what is not separated.

Schools data Ozone data

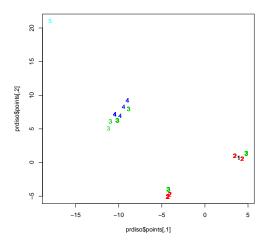
3 Data analysis 3.1 Schools data

MDS on fit distance (with clustering)



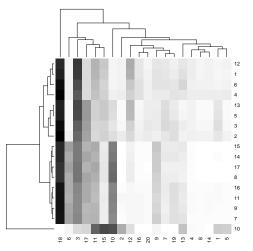
Schools data Ozone data

Where are best models?



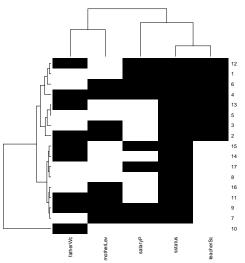
Schools data Ozone data

Models and squared residuals



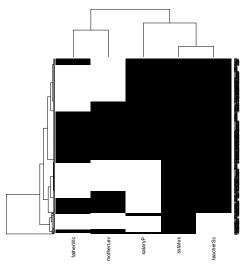
Schools data Ozone data

Models and variables



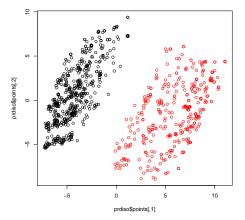
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Models and variables (by bootstrap run)



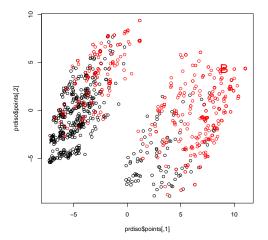
Schools data Ozone data

3.2 Ozone data MDS on fit distance with clusters



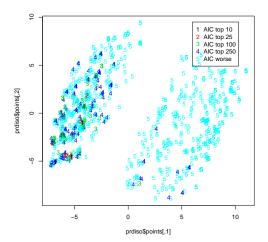
Schools data Ozone data

Models found by AIC, BIC



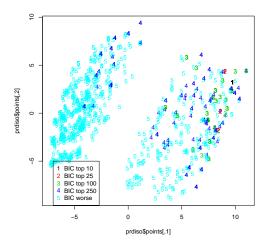
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Best AIC



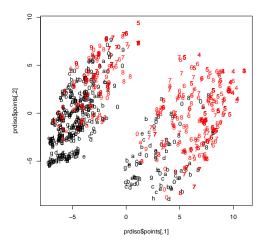
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Best BIC



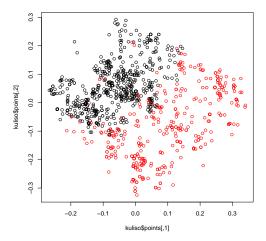
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Size of models



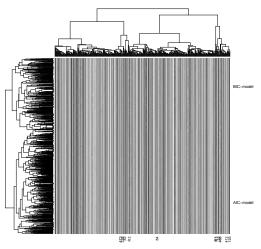
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Variable-based distance (with clusters from before)



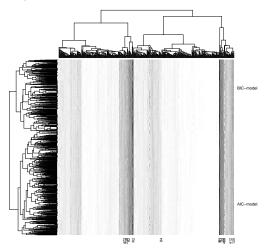
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Models and fits



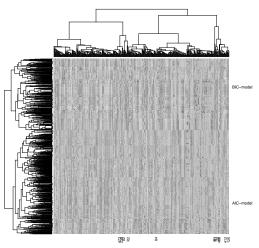
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Models and squared residuals



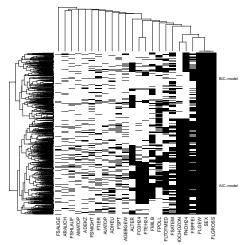
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Models and squared residuals (column standardised)



Schools data Ozone data

Models and variables



Variables that make a difference can clearly be seen.

Christian Hennig, Willi Sauerbrei Exploration of bootstrapped variable selection



4 What we learnt

Large variability in models for both datasets.

Schools data:

- Four clusters of models deliver quite different fits.
- Some models fit some (~ half) points very well, disregarding others.
- Better AIC achieved by "compromise fits" (including TeacherSc variable).



Ozone data

- Two clusters of model fits, not aligned with BIC/AIC-models, rather connected to vars HOCHOZON, FNOH24 and FN3H24.
- BIC- and AIC-selected models are quite different.
- Little variation between model fits and residuals, choice between them somewhat arbitrary.



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Not shown: atypicality of models,

and observations supporting atypical models.

A bit of marketing:

Chapman & Hall/CRC Handbooks of Modern Statistical Methods

Handbook of Cluster Analysis

Edited by Christian Hennig Marina Meila Fionn Murtagh Roberto Rocci

CRC Press

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