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Shluková analýza ve směsích regresních modelů

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Standard mixture regression models

- Standard linear regression model

$$y_j = \mathbf{x}_j^{\mathrm{T}} \boldsymbol{\beta} + \varepsilon_j$$

- The mixture of linear regression models can be written as

$$y_j = \begin{cases} \mathbf{x}_j^{\mathrm{T}} \boldsymbol{\beta}_1 + \varepsilon_{1j} & \text{with probability } \pi_1 \\ \mathbf{x}_j^{\mathrm{T}} \boldsymbol{\beta}_2 + \varepsilon_{2j} & \text{with probability } \pi_2 \\ & \vdots \\ \mathbf{x}_j^{\mathrm{T}} \boldsymbol{\beta}_c + \varepsilon_{cj} & \text{with probability } \pi_c \end{cases} \qquad \text{where } \varepsilon_{ij} \sim \mathrm{N}(0, \sigma_i^2)$$

- Accounting for the mixture structure, the conditional density of $y_j | \mathbf{x}_j$ is

$$f(y_j | \mathbf{x}_j, \boldsymbol{\Psi}) = \sum_{i=1}^{c} \pi_i \phi(y_j | \mathbf{x}_j^{\mathrm{T}} \boldsymbol{\beta}_i, \sigma_i^2).$$

- $\boldsymbol{\Psi}$ denotes the vector of all parameters

$$\boldsymbol{\Psi} = (\pi_1, \ldots, \pi_c, (\boldsymbol{\beta}_1^{\mathrm{T}}, \sigma_1^2), \ldots, (\boldsymbol{\beta}_c^{\mathrm{T}}, \sigma_c^2))^{\mathrm{T}}.$$

- Maximizing the log likelihood function

$$\log L(\boldsymbol{\Psi}|\mathbf{x}_1,\ldots,\mathbf{x}_n,y_1,\ldots,y_n)=\sum_{j=1}^{n}\log\left(\sum_{i=1}^{c}\pi_i\phi(y_j|\mathbf{x}_j^{\mathrm{T}}\boldsymbol{\beta}_i,\sigma_i^2)\right).$$

- The **EM algorithm** is an iterative procedure which alternates between an Expectation step and a Maximization step.

$(k+1)$th iteration of EM algorithm:

1. **E-step**: Given the observed data $\mathbf{y}$ and current parameter estimates $\widehat{\boldsymbol{\Psi}}^{(k)}$ in the kth iteration, calculates estimated a-posteriori probabilities, assigning each observation j to each cluster i.

$$\widehat{\tau}_{ij}^{(k)}=\frac{\widehat{\pi}_i^{(k)}\phi(y_j|\mathbf{x}_j^{\mathrm{T}}\widehat{\boldsymbol{\beta}}_i^{(k)},\widehat{\sigma}_i^{2(k)})}{\sum_{h=1}^{c}\widehat{\pi}_h^{(k)}\phi(y_j|\mathbf{x}_j^{\mathrm{T}}\widehat{\boldsymbol{\beta}}_h^{(k)},\widehat{\sigma}_h^{2(k)})}.$$

2. **M-step**: Given the estimates $\widehat{\tau}_{ij}^{(k)}$ for the a-posteriori probabilities τ_{ij} (which are functions of $\widehat{\boldsymbol{\Psi}}^{(k)}$), obtain new estimates $\widehat{\boldsymbol{\Psi}}^{(k+1)}$ of the parameters by maximizing expected complete log–likelihood, which is in general easier to maximize than the original likelihood.

$$Q(\boldsymbol{\Psi},\widehat{\boldsymbol{\Psi}}^{(k)})=\sum_{j=1}^{n}\sum_{i=1}^{c}\widehat{\tau}_{ij}^{(k)}\log\phi(y_j|\mathbf{x}_j^{\mathrm{T}}\boldsymbol{\beta}_i,\sigma_i^2)$$

- The maximization is equivalent to solving the weighted least squares problem:

$$\widehat{\boldsymbol{\beta}}_i^{(k+1)} = (\mathbf{X}^{\mathrm{T}}\mathbf{W}_i^{(k)}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{W}_i^{(k)}\mathbf{y} \qquad \text{for} \quad i = 1, \ldots, c,$$

  where $\mathbf{y} = (y_1, \ldots, y_n)^T$ is the vector of observations and $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)^T$ is the design matrix, both are weighted by $\widehat{\tau}_{ij}^{\,1/2\,(k)}$.

- In order to estimate $\widehat{\sigma}_i^2$ and $\widehat{\pi}_i$ we use

$$\widehat{\sigma}^{2\,(k+1)} = \frac{(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_i^{(k+1)})^{\mathrm{T}}\mathbf{W}_i(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_i^{(k+1)})}{n}, \qquad \text{for} \quad i = 1, \ldots, c,$$

- and

$$\widehat{\pi}_i^{(k+1)} = \frac{\sum_{j=1}^n \tau_{ij}^{(k)}}{n} \qquad \text{for} \quad i = 1, \ldots, c.$$

Mixture regression models with concomitant variables

- We consider mixture of regressions with concomitant variables of form

$$f(y_j|\mathbf{x}_j, \boldsymbol{\omega}_j) = \sum_{i=1}^{c} \pi_i(\boldsymbol{\omega}_j, \boldsymbol{\alpha}_i)\phi(y_j|\mathbf{x}_j^{\mathrm{T}}\boldsymbol{\beta}_i, \sigma_i^2),$$

- Multinomial logit model for the π_i is given by

$$\pi_i(\boldsymbol{\omega}_j, \boldsymbol{\alpha}_i) = \frac{\exp^{\boldsymbol{\omega}_j^{\mathrm{T}}\boldsymbol{\alpha}_i}}{\sum_{h=1}^{c}\exp^{\boldsymbol{\omega}_j^{\mathrm{T}}\boldsymbol{\alpha}_h}} \qquad \text{for} \qquad i = 1, \ldots, c,$$

with $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_c)$ and $\boldsymbol{\alpha}_1 \equiv \mathbf{0}$.
- The vector of all parameters is given by

$$\boldsymbol{\Psi} = ((\boldsymbol{\alpha}_1^{\mathrm{T}}, \boldsymbol{\beta}_1^{\mathrm{T}}, \sigma_1^2), \ldots, (\boldsymbol{\alpha}_c^{\mathrm{T}}, \boldsymbol{\beta}_c^{\mathrm{T}}, \sigma_c^2))^{\mathrm{T}}.$$

- Parameters estimated via EM algorithm.
- M-step: maximization of expected complete log likelihood

$$Q(\boldsymbol{\Psi}, \widehat{\boldsymbol{\Psi}}^{(k)}) = Q_1(\boldsymbol{\beta}_i, \sigma_i^2, i = 1, \ldots, c\,; \widehat{\boldsymbol{\Psi}}^{(k)}) + Q_2(\boldsymbol{\alpha}, \widehat{\boldsymbol{\Psi}}^{(k)}),$$

where

$$Q_1(\boldsymbol{\beta}_i, \sigma_i^2, i = 1, \ldots, c\,; \widehat{\boldsymbol{\Psi}}^{(k)}) = \sum_{j=1}^{n} \sum_{i=1}^{c} \widehat{\tau}_{ij}^{(k)} \log\left(\phi(y_j | \mathbf{x}_j^{\mathrm{T}} \boldsymbol{\beta}_i, \sigma_i^2)\right)$$

and

$$Q_2(\boldsymbol{\alpha}, \widehat{\boldsymbol{\Psi}}^{(k)}) = \sum_{j=1}^{n} \sum_{i=1}^{c} \widehat{\tau}_{ij}^{(k)} \log\left(\pi_i(\boldsymbol{\omega}_j, \boldsymbol{\alpha}_i)\right).$$

- Formulas Q_1 and Q_2 can be maximized separately. The maximization of Q_1 gives new estimates $\widehat{\boldsymbol{\beta}}_i^{(k+1)}, \widehat{\sigma}_i^{2(k+1)}$, $i = 1, \ldots, c$, and the maximization of Q_2 gives $\widehat{\boldsymbol{\alpha}}^{(k+1)}$. Q_1 is maximized using the weighted ML estimation of linear models and Q_2 by means of the weighted ML estimation of multinomial logit models.

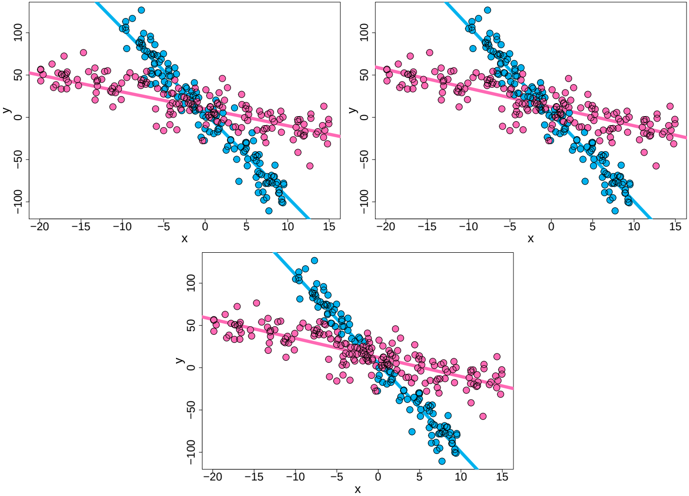
Categorical concomitant variable

- The data comes from two component mixture of the following structure:

$$
\begin{aligned}
150\,\mathrm{obs.}: \quad & y = 5 - 10\,x + \varepsilon; \qquad & \varepsilon \sim \mathrm{N}(0, 15) \\
150\,\mathrm{obs.}: \quad & y = 10 - 2\,x + \varepsilon; \qquad & \varepsilon \sim \mathrm{N}(0, 15)
\end{aligned}
$$

- Categorical concomitant variable assigns value 1 and 2 to observations from the first component (with accuracy of 90%) and value 3 and 4 to observations from the second component (with accuracy of 90%)

- Comparison of true data classification (top left), classification via ordinary mixture of regressions (bottom) and classification via mixture of regressions with concomitant variable (top right).



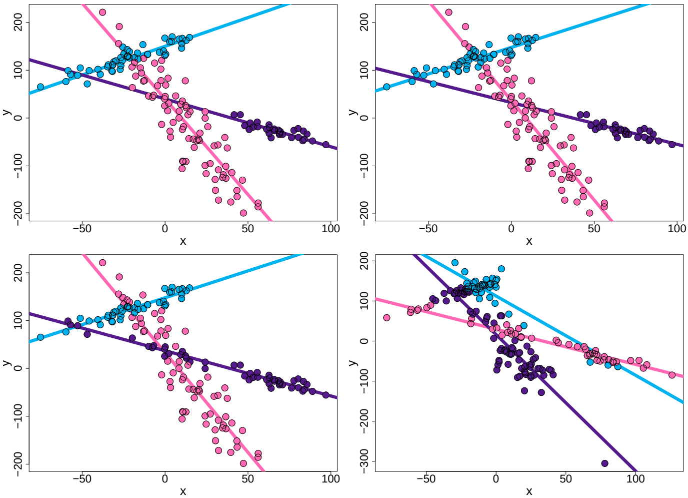
Continuous concomitant variable

- The data comes from three component mixture of the following structure:

$$\begin{array}{lll} 50\,\text{obs.}: & y = 150 - 1.2\,x + \varepsilon; & \varepsilon \sim \mathrm{N}(0,10) \\ 80\,\text{obs.}: & y = 40 - 4\,x + \varepsilon; & \varepsilon \sim \mathrm{N}(0,40) \\ 30\,\text{obs.}: & y = 40 - 1\,x + \varepsilon; & \varepsilon \sim \mathrm{N}(0,10) \end{array}$$

- Explanatory variable can be used as concomitant variable for better estimates of observations membership.

- Comparison of true data classification (top left), classification via ordinary mixture of regressions (bottom left & bottom right) and classification via mixture of regressions with concomitant variable (top right).



- The *MSE* and variance of the regression parameters and standard error estimates for both mixture models:

$MSEPAR(\widehat{\psi}_m)$	β_{10}	β_{11}	β_{20}	β_{21}	β_{10}	β_{11}	β_{20}	β_{21}	β_{30}	β_{31}
klasická směs	2.098	0.095	2.189	0.023	5.508	0.006	55.368	0.069	149.421	0.028
směs s dopr. prom.	**1.763**	**0.057**	**1.809**	**0.017**	**5.017**	0.006	**30.709**	**0.059**	**61.040**	**0.011**
$VAR(\widehat{\psi}_m)$	β_{10}	β_{11}	β_{20}	β_{21}	β_{10}	β_{11}	β_{20}	β_{21}	β_{30}	β_{31}
klasická směs	2.033	0.051	2.063	0.018	**3.683**	0.005	34.297	0.059	**13.816**	**0.003**
směs s dopr. prom.	**1.713**	**0.048**	**1.799**	**0.016**	4.772	0.005	**29.577**	0.059	56.016	0.010

- For three component mixture - most of the standard mixture estimates are completely inaccurate and not included in the estimates quality comparison.

Conclusions

- Mixtures of regression models can be applied to data where observations originate from various groups and the group affiliations are not known.
- Mixture of regressions with concomitant variables provides quality estimates in the sense of lower MSE and variance of parameters.
- Concomitant variable enhances the classification of observations.

Thank you for your attention!

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