Robust variable selection for model-based learning from adulterated samples

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joint work with **Francesca Greselin** and **Brendan Murphy**

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Outline

1. Chemometric contest
2. Feature selection in classification
3. Robust model-based Discriminant Analysis
4. Robust variable selection
    - Stepwise greedy-forward approach via TBIC
    - ML subset selector approach
5. Starches discrimination
6. Open Problems and Future Research

Chemometric contest

- MIR spectra of starches of four different classes (Fernández Pierna and Dardenne 2007)
- $P = 2901$ absorbance measurements for each sample
- Training and test sets of $N = 215$ and $M = 43$ units, respectively
- Adulterated samples (more details later!)

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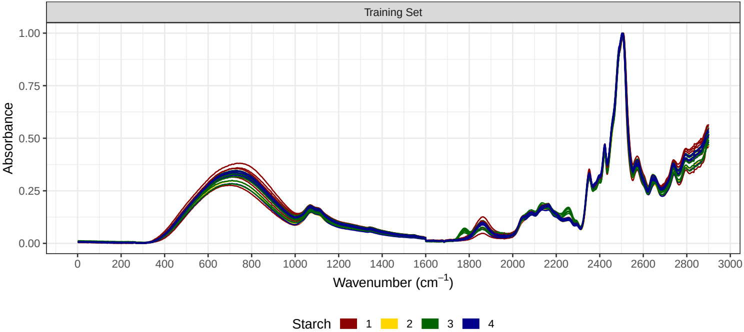

Motivating problem

Classification framework:

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- Contaminated units (label noise and modifications)

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Model-based method with variable selection would be optimal, but attribute and class noise can heavily damage the performance of standard methods (Zhu and Wu 2004)!

Variable selection in classification

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The detection of p relevant features (out of $P >> p$) is particularly desirable as (McLachlan 1992):

- it simplifies parameters estimation and interpretation
- it avoids loss on predictive power
- it leads to cost reduction on future data collection
- it mitigates the *curse of dimensionality* (Bellman 1957) in model-based methods
- for MIR spectra, adjacent wavelengths are often correlated and virtually contain the same information (Indahl and Næs 2004)

Variables role in DA

- *Relevant variables*: their distribution directly depends on the class membership
- *Irrelevant or noisy variables*: their distribution is completely independent from the group structure
- *Redundant variables*: their distribution is conditionally independent on the class membership, given the relevant features

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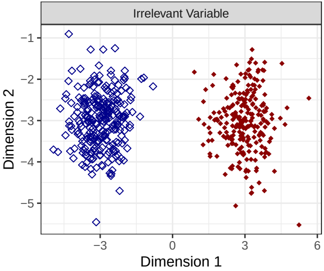

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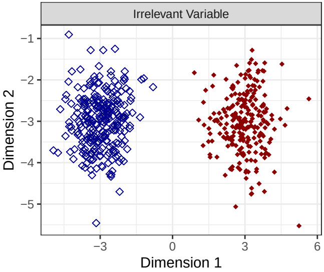

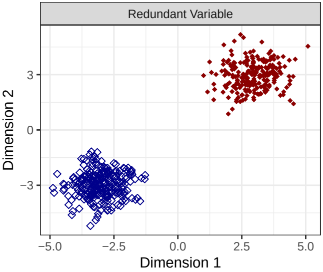

Robust Model-Based Classification

- A complete set of N learning observations:

$$(\mathbf{x}, \mathbf{l}) = \left\{ (\mathbf{x}_1, \mathbf{l}_1), \dots, (\mathbf{x}_N, \mathbf{l}_N); \mathbf{x}_n \in \mathbb{R}^P, l_n \in \{1, \dots, G\} \right\}$$

$\mathbf{x}_n$ is a P-dimensional predictor and $\mathbf{l}_n$ its associated label

- Data generating process for **genuine** observations

$$\mathcal{G} \sim Mult_G(1; \tau_1, \dots, \tau_G) \quad \mathcal{X} | \mathcal{G} = g \sim \mathcal{N}_P(\boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g)$$

$$p(\mathbf{x}_n, \mathbf{l}_n; \boldsymbol{\theta}) = p(\mathbf{l}_n; \boldsymbol{\tau}) p(\mathbf{x}_n | \mathbf{l}_n = g; \boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g) = \prod_{g=1}^{G} \left[\tau_g \phi(\mathbf{x}_n; \boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g) \right]^{l_{ng}}$$

  - $\phi(\cdot; \boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g)$ multivariate normal density distribution
  - τ_g prior probability of the gth class
  - $\boldsymbol{\Sigma}_g = \lambda_g \boldsymbol{D}_g \boldsymbol{A}_g \boldsymbol{D}_g'$ (Bensmail and Celeux 1996)

Robust Model-Based Classification

REDDA protects the estimates against label noise and outliers defining a suitable trimmed mixture log-likelihood (Cappozzo, Greselin, and Murphy 2019)

$$\ell_{trim}(\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma}|\mathbf{X}, \mathbf{l}) = \sum_{n=1}^{N} \zeta(\mathbf{x}_n) \sum_{g=1}^{G} \mathrm{l}_{ng} \log \left(\tau_g \phi(\mathbf{x}_n; \boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g)\right) \quad (1)$$

- $\zeta(\cdot)$ 0-1 trimming indicator function
- α_l *labelled trimming level*: $\sum_{n=1}^{N} \zeta(\mathbf{x}_n) = \lceil N(1-\alpha_l) \rceil$
- (1) maximized via a generalization of the FastMCD algorithm (Rousseeuw and Driessen 1999)
- *Concentration step* discards $\lfloor N\alpha_l \rfloor$% units with lowest:

$$f(\mathbf{x}_n | l_{ng} = 1; \hat{\boldsymbol{\mu}}_g, \hat{\boldsymbol{\Sigma}}_g) = \phi\left(\mathbf{x}_n; \hat{\boldsymbol{\mu}}_g, \hat{\boldsymbol{\Sigma}}_g\right) \qquad n = 1, \ldots, N.$$

Robust variable selection

Two proposals for robust variable selection in model-based classification

Robust variable selection

Two proposals for robust variable selection in model-based classification

- Robust stepwise greedy-forward approach via TBIC
  - Robust classification rule built in a step-wise manner
  - TBIC used for model comparison
  - Automatic selection of the relevant subset size

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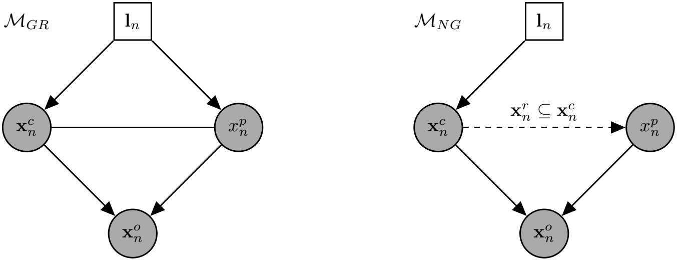
- ML subset selector approach
  - Based on MLE theory and irrelevance in Gaussian mixtures
  - Relevant subset as a parameter to be estimated via ML
  - Relevant subset size is a-priori specified

Robust stepwise via TBIC

At each step of the algorithm, the learning observations are partitioned as $\mathbf{x}_n = (\mathbf{x}_n^c, x_n^p, \mathbf{x}_n^o)$ (Raftery and Dean 2006):

- $\mathbf{x}_n^c$ the variables currently included in the model
- x_n^p the variable proposed for inclusion
- $\mathbf{x}_n^o$ the remaining variables



Grouping

$p(\mathbf{x}_n^c, x_n^p|\mathbf{l}_n)p(\mathbf{x}_n^o|x_n^p, \mathbf{x}_n^c)$

No Grouping

$p(\mathbf{x}_n^c|\mathbf{l}_n)p(x_n^p|\mathbf{x}_n^r \subseteq \mathbf{x}_n^c)p(\mathbf{x}_n^o|x_n^p, \mathbf{x}_n^c)$

Robust stepwise via TBIC

Model comparison is carried out employing a robust approximation to the Bayes Factor (Kass and Raftery 1995):

$$\mathcal{B}_{GR,NG} = \frac{p(\mathbf{x}_n|\mathcal{M}_{GR})}{p(\mathbf{x}_n|\mathcal{M}_{NG})} = \frac{\int p(\mathbf{x}_n|\boldsymbol{\theta}_{GR}, \mathcal{M}_{GR}) p(\boldsymbol{\theta}_{GR}|\mathcal{M}_{GR}) d\boldsymbol{\theta}_{GR}}{\int p(\mathbf{x}_n|\boldsymbol{\theta}_{NG}, \mathcal{M}_{NG}) p(\boldsymbol{\theta}_{NG}|\mathcal{M}_{NG}) d\boldsymbol{\theta}_{NG}}$$

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Trimmed BIC (Neykov et al. 2007), is employed as a robust proxy for the integrated likelihoods

$$2\log\left(\mathcal{B}_{GR,NG}\right) \approx TBIC(Grouping) - TBIC(No\ Grouping) \qquad (2)$$

Variable x_n^p with a positive difference in (2) is a candidate for being added (removed) to (from) the model

Robust stepwise via TBIC

$$TBIC(GR) = \underbrace{2\sum_{n=1}^{N}\zeta(\mathbf{x}_n^c, x_n^p)\sum_{g=1}^{G}\mathfrak{l}_{ng}\log\left(\hat{\tau}_g^{cp}\phi(\mathbf{x}_n^c, x_n^p; \hat{\boldsymbol{\mu}}_g^{cp}, \hat{\boldsymbol{\Sigma}}_g^{cp})\right)}_{2\times\text{trimmed log maximized likelihood of } p(\mathbf{x}_n^c, x_n^p, \mathbf{l}_n)} +$$

$$- v^{cp} log(N^*)$$

$$TBIC(NG) = \underbrace{2\sum_{n=1}^{N}\iota(\mathbf{x}_n^c, x_n^p)\sum_{g=1}^{G}\mathfrak{l}_{ng}\log\left(\hat{\tau}_g^{c}\phi(\mathbf{x}_n^c; \hat{\boldsymbol{\mu}}_g^{c}, \hat{\boldsymbol{\Sigma}}_g^{c})\right)}_{2\times\text{trimmed log maximized likelihood of } p(\mathbf{x}_n^c, \mathbf{l}_n)} - v^c log(N^*) +$$

$$\underbrace{+2\sum_{n=1}^{N}\iota(\mathbf{x}_n^c, x_n^p)\log\left[\phi\left(x_n^p; \hat{\alpha} + \hat{\boldsymbol{\beta}}'\mathbf{x}_n^r, \hat{\sigma}^2\right)\right]}_{2\times\text{trimmed log maximized likelihood of } p(x_n^p|\mathbf{x}_n^r\subseteq\mathbf{x}_n^c)} - v^p log(N^*).$$

ML subset selector

A model for the entire P-dimensional space is built:

- $F \subseteq 1, \ldots, P$ set of relevant variables, $|F| = p$
- $E = \bar{F}$ set of irrelevant variables, $|E| = P - p$

Exploiting the theory for the multivariate Gaussian under irrelevance (Ritter 2014)

$$\ell_{trim}(\boldsymbol{\tau}, \boldsymbol{\mu}_F, \boldsymbol{\Sigma}_F, \boldsymbol{G}_{E|F}, \boldsymbol{\mu}_{E|F}, \boldsymbol{\Sigma}_{E|F} | \mathbf{X}, \mathbf{l}) =$$

$$= \sum_{n=1}^{N} \zeta(\mathbf{x}_n) \left(\sum_{g=1}^{G} l_{ng} \log \left[\tau_g \phi(\mathbf{x}_{n,F}; \boldsymbol{\mu}_{g,F}, \boldsymbol{\Sigma}_{g,F}) \right] + \right.$$

$$\left. + \log \left[\phi(\mathbf{x}_{n,E} - \boldsymbol{G}_{E|F} \mathbf{x}_{n,F}; \boldsymbol{\mu}_{E|F}, \boldsymbol{\Sigma}_{E|F}) \right] \right)$$

$$\boldsymbol{\mu}_{E|F} = \boldsymbol{\mu}_E - \boldsymbol{G}_{E|F} \boldsymbol{\mu}_F, \quad \boldsymbol{\Sigma}_{E|F} = \boldsymbol{\Sigma}_E - G_{E|F} \boldsymbol{\Sigma}_{F,E}, \quad \boldsymbol{G}_{E|F} = \boldsymbol{\Sigma}_{E,F} \boldsymbol{\Sigma}_F^{-1}$$

ML subset selector

1. *Robust Initialization:*
   - Draw a random $(P+1)$-subset for each class g, $g = 1, \ldots, G$
   - $\zeta(\mathbf{x}_n) = 1$ if $\mathbf{x}_n$ belongs to any of such G subsets, otherwise $\zeta(\mathbf{x}_n) = 0$ (different strategy if $P >> p$)
2. *M-step:*

$$\hat{\tau}_g = \frac{\sum_{n=1}^{N} \zeta(\mathbf{x}_n) l_{ng}}{\lceil N(1-\alpha_l) \rceil} \quad g = 1, \ldots, G$$

$$\hat{\boldsymbol{\mu}}_g = \frac{\sum_{n=1}^{N} \zeta(\mathbf{x}_n) l_{ng} \mathbf{x}_n}{\sum_{n=1}^{N} \zeta(\mathbf{x}_n) l_{ng}} \quad g = 1, \ldots, G.$$

$$\hat{\boldsymbol{\mu}} = \frac{\sum_{n=1}^{N} \zeta(\mathbf{x}_n) \mathbf{x}_n}{\lceil N(1-\alpha_l) \rceil}.$$

$\hat{\boldsymbol{\Sigma}}_g$ and $\hat{\boldsymbol{\Sigma}}$ according to (Bensmail and Celeux 1996)

ML subset selector

3. *S-step:* Minimize the difference

$$h(F) = \sum_{g=1}^{G} \hat{\tau}_g \log \det \hat{\boldsymbol{\Sigma}}_{g,F} - \log \det \hat{\boldsymbol{\Sigma}}_F$$

w.r.t. the subset $\hat{F} \subseteq 1, \ldots, P$

4. *T-step:*

$$\hat{\boldsymbol{G}}_{\hat{E}|\hat{F}} = \hat{\boldsymbol{\Sigma}}_{\hat{E},\hat{F}} \hat{\boldsymbol{\Sigma}}_{\hat{F}}^{-1}, \;\; \hat{\boldsymbol{\mu}}_{\hat{E}|\hat{F}} = \hat{\boldsymbol{\mu}}_{\hat{E}} - \hat{\boldsymbol{G}}_{\hat{E}|\hat{F}} \hat{\boldsymbol{\mu}}_{\hat{F}}, \;\; \hat{\boldsymbol{\Sigma}}_{\hat{E}|\hat{F}} = \hat{\boldsymbol{\Sigma}}_{\hat{E}} - \hat{\boldsymbol{\Sigma}}_{\hat{E},\hat{F}} \hat{\boldsymbol{\Sigma}}_{\hat{F}}^{-1} \hat{\boldsymbol{\Sigma}}_{\hat{F},\hat{E}}$$

Update the value of $\zeta(\cdot)$, discarding $\lfloor N\alpha_l \rfloor$% units with lowest:

$$\sum_{g=1}^{G} l_{ng} \log \left[\hat{\tau}_g \phi(\mathbf{x}_{n,\hat{F}}; \hat{\boldsymbol{\mu}}_{g,\hat{F}}, \hat{\boldsymbol{\Sigma}}_{g,\hat{F}}) \right] + \log \left[\phi \left(\mathbf{x}_{n,\hat{E}} - \hat{\boldsymbol{G}}_{\hat{E}|\hat{F}} \mathbf{x}_{n,\hat{F}}; \hat{\boldsymbol{\mu}}_{\hat{E}|\hat{F}}, \hat{\boldsymbol{\Sigma}}_{\hat{E}|\hat{F}} \right) \right]$$

5. Iterate $2 - 4$ until $\zeta(\cdot)$ does not change.

Data adulteration

- Training set: 4 units with label noise

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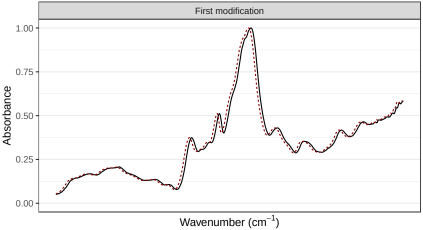

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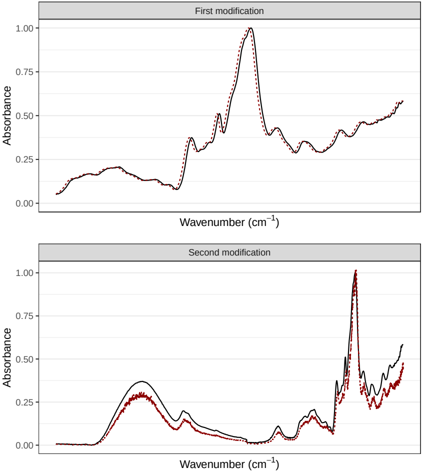

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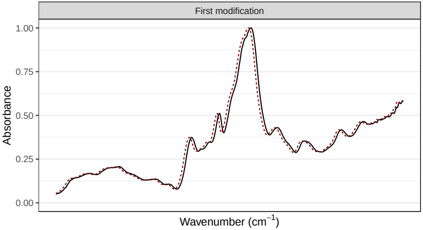

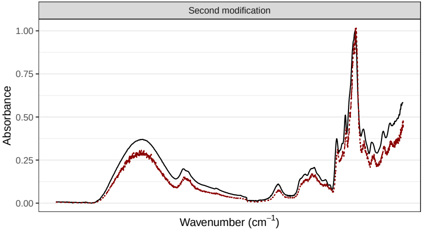

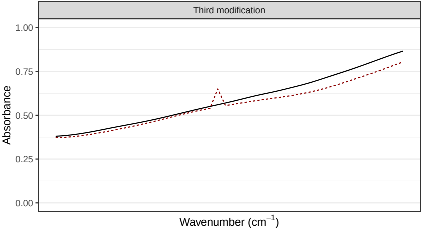

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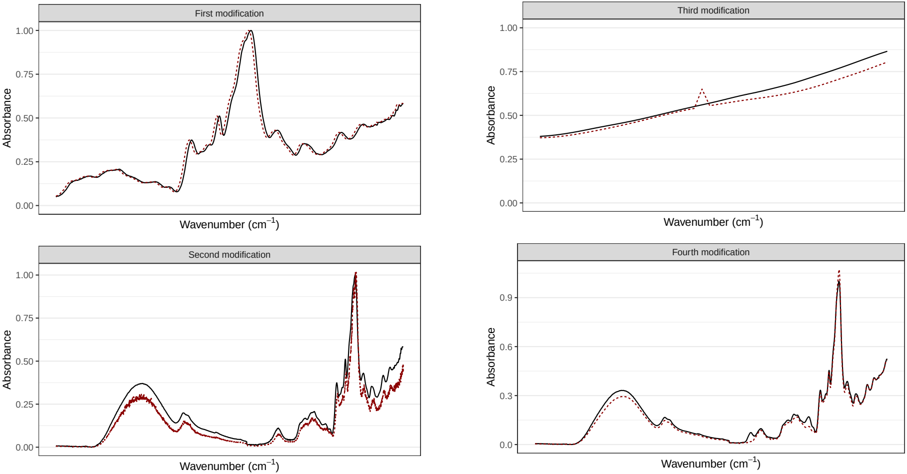
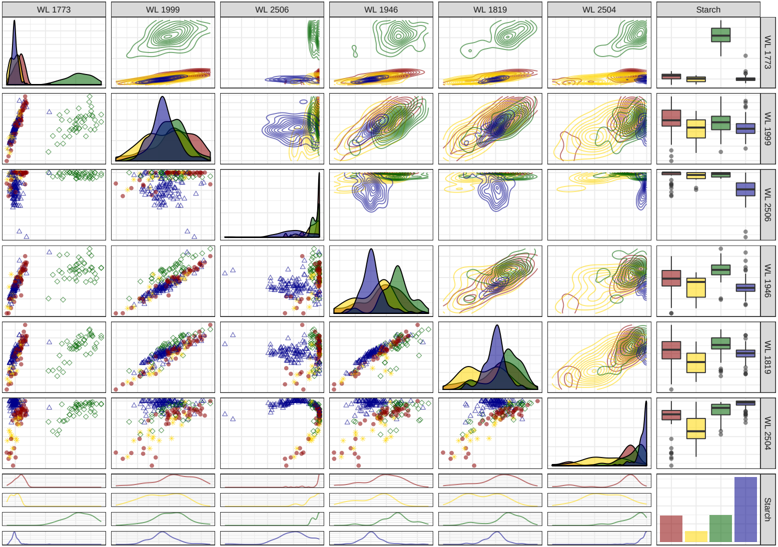


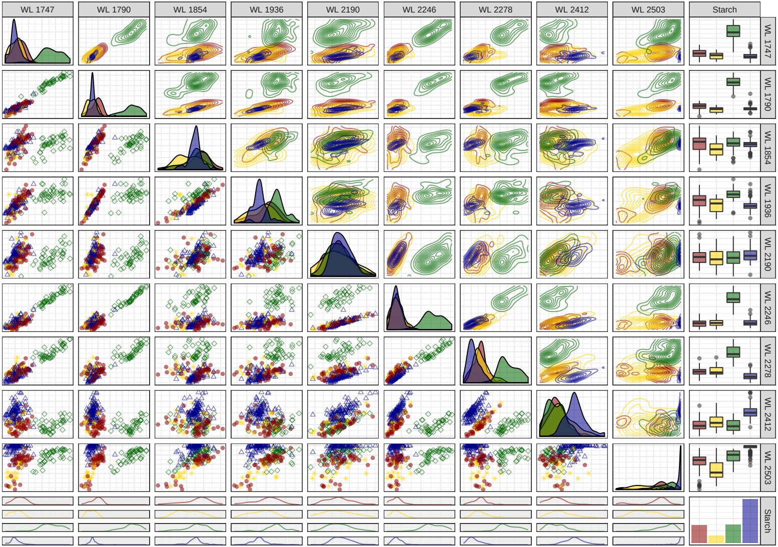
Results: Robust stepwise via TBIC

Selected WL: 1773, 1999, 2506, 1946, 1819, 2504



Results: ML subset selector

Selected WL: 1747, 1790, 1854, 1936, 2190, 2246, 2278, 2412, 2503



Results & adulteration detection

	REDDA (TBIC)	REDDA (ML subset)	SVM radial kernel	ROC+PLS+SVM
With outliers				
# correctly predicted	34	36	32	33
% correctly predicted	0.791	0.837	0.744	0.767
Without outliers				
#correctly predicted	32	34	31	31
% correctly predicted	0.821	0.872	0.795	0.795

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- Adulteration detection is performed considering:

$$\hat{p}(\mathbf{y}_{m,\hat{F}}; \hat{\tau}, \hat{\boldsymbol{\mu}}_{\hat{F}}, \hat{\boldsymbol{\Sigma}}_{\hat{F}}) = \sum_{g=1}^{G} \hat{\tau}_g \phi\left(\mathbf{y}_{m,\hat{F}}; \hat{\boldsymbol{\mu}}_{g,\hat{F}}, \hat{\boldsymbol{\Sigma}}_{g,\hat{F}}\right) \tag{3}$$

3 out of the 4 modified units possess lowest values of (3).

Conclusions

We have introduced two wrapper variable selection methods, resistant to outliers and label noise

- Robust stepwise via TBIC: robust model-based classifier within a greedy-forward algorithm
- ML subset selector: the subset of relevant variables is a parameter to be estimated

Future research direction

- Extension to the adaptive framework, where unobserved classes in the test set need to be discovered
- Development of dedicated R package

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Thank You!