A Robust Approach to Regularized Discriminant Analysis

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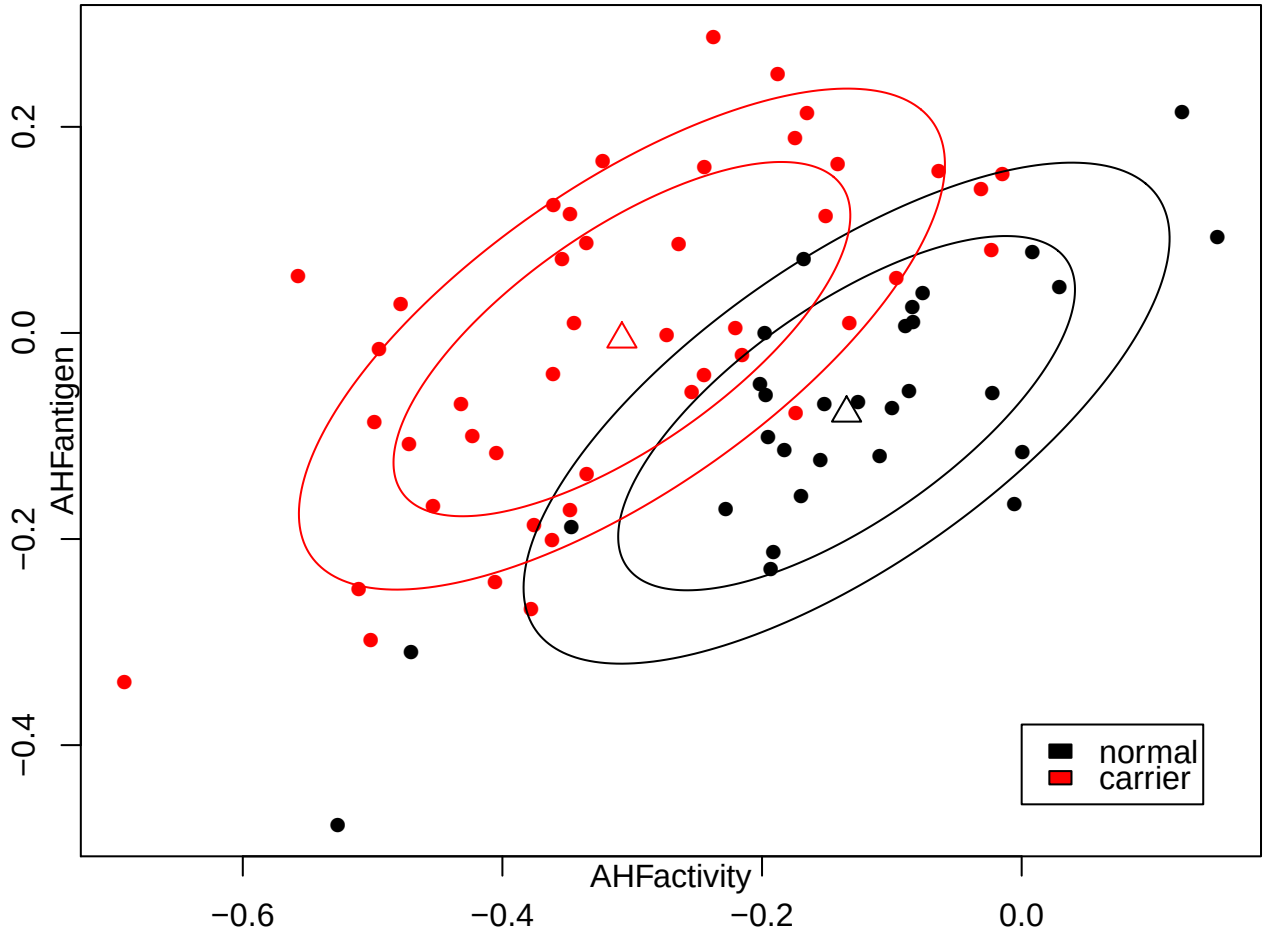
Discriminant Analysis (DA): Example

Haemophilia data: 30 normal persons and 22 obligatory carriers of hemophilia A



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Notation

Given n observations of training data, measured at p variables.

Observations originate from

- k different populations $G_1, \ldots, G_k$,
- according to prior probabilities $\pi_1, \ldots, \pi_k$, where $\sum_{j=1}^{k} \pi_j = 1$,
- with sample sizes $n_1, \ldots, n_k$, where $\sum_{j=1}^{k} n_j = n$.
- **Usual assumption:** Observations are distributed according to a normal distribution $\mathbf{N}(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$, with mean $\boldsymbol{\mu}_j$ and covariance matrix $\boldsymbol{\Sigma}_j$, $j = 1, \ldots, k$.

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DA: Classification and Prediction

Find a classification function f based on the training data that assigns a new, unlabelled observation to one (and only one) of the k groups:

$$f : \Omega^p \to \{1, \ldots, k\}$$

Bayes Rule: Given an observation $\boldsymbol{x}$, the posterior probability for group G_j equals

$$P(G_j|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|G_j) \cdot \pi_j}{\sum_{i=1}^{k} p(\boldsymbol{x}|G_i) \cdot \pi_i}$$

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Bayesian DA Rule

A **test set observation** $\boldsymbol{x}$ is assigned to that population G_j, for which $\ln P(G_j|\boldsymbol{x})$ is a maximum over all groups $j = 1, \ldots, k$.

$$\Rightarrow f(\boldsymbol{x}) = \arg\max_j \Big(\ln(P(G_j|\boldsymbol{x}))\Big) = \arg\max_j \Big(\ln(p(\boldsymbol{x}|G_j) \cdot \pi_j)\Big)$$

Quadratic Discriminant Analysis:

$$f_{QDA}(\boldsymbol{x}) = \arg\max_j \left(-\frac{1}{2}\ln(\det \boldsymbol{\Sigma}_j) - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_j)^\top \boldsymbol{\Sigma}_j^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_j) + \ln \pi_j\right)$$

Linear Discriminant Analysis: assume $\boldsymbol{\Sigma}_1 = \ldots = \boldsymbol{\Sigma}_k = \boldsymbol{\Sigma}$, and use

$$f_{LDA}(\boldsymbol{x}) = \arg\max_j \left(\boldsymbol{\mu}_j^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{x} - \frac{1}{2}\boldsymbol{\mu}_j^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_j + \ln \pi_j\right)$$

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Parameter Estimation

The essential elements of the LDA rule are the group centers and the common group covariance matrix.

Estimate **group centers** and the **common group covariance matrix** by

- the sample means and pooled sample covariance matrix.
- **robust estimators** of location and covariance, like the MCD estimators.
- **regularized (sparse)** estimators of location and covariance.

Robust estimators lead to robust DA rules!

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Maximum Likelihood

Given a data sample $\mathbf{X}$, the log-likelihood function of joint location $\boldsymbol{\mu}$ and inverse scatter $\boldsymbol{\Theta} := \boldsymbol{\Sigma}^{-1}$ is given by

$$\mathcal{L}(\boldsymbol{\mu}, \boldsymbol{\Theta}) = \log(\det(\boldsymbol{\Theta})) - \frac{1}{n} \sum_{\boldsymbol{x} \in \mathbf{X}} (\boldsymbol{x} - \boldsymbol{\mu})^\top \boldsymbol{\Theta} (\boldsymbol{x} - \boldsymbol{\mu})$$

$\Rightarrow$ Maximization leads to **classical estimators:**

$$\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_{\boldsymbol{x} \in \mathbf{X}} \boldsymbol{x}$$

$$\hat{\boldsymbol{\Theta}} = \hat{\boldsymbol{\Sigma}}^{-1} = (\frac{1}{n} \sum_{\boldsymbol{x} \in \mathbf{X}} (\boldsymbol{x} - \hat{\boldsymbol{\mu}})(\boldsymbol{x} - \hat{\boldsymbol{\mu}})^\top)^{-1}$$

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Regularization

Problem: If $n < p$, $\hat{\Sigma}$ is singular and the maximum likelihood estimator for Θ does not exist!

Solution: Penalization of log-likelihood function based on penalty term $\lambda > 0$ and L1 Norm $\|.\|_1$:

$$\mathcal{L}(\boldsymbol{\mu}, \Theta) = \log(\det(\Theta)) - \frac{1}{n} \sum_{\boldsymbol{x} \in \mathbf{X}} (\boldsymbol{x} - \boldsymbol{\mu})^\top \Theta (\boldsymbol{x} - \boldsymbol{\mu}) - \lambda \|\Theta\|_1$$

$$\|\Theta\|_1 = \sum_{l,m} |\theta_{lm}|$$

The maximization problem can be solved by an algorithm called graphical lasso. λ governs sparseness of $\hat{\Sigma}$ and $\hat{\Theta}$!

package: `glasso` (Friedman, Hastie, Tibshirani, 2007).

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Example

Simulated three-dimensional data, $\mathbf{X} \sim \mathbf{N}(\mathbf{0}, \mathbf{I}_3), n = 100$:

```
> solve(cov(X))
       [,1]   [,2]   [,3]
[1,]  1.179 -0.039 -0.088
[2,] -0.039  0.835 -0.147
[3,] -0.088 -0.147  1.100

> glasso(cov(X), rho=0.2)$wi
      [,1] [,2]  [,3]
[1,] 0.948  0.0 0.000
[2,] 0.000  0.7 0.000
[3,] 0.000  0.0 0.879
```

$\lambda = 0.2$ leads to **sparse estimate** of concentration matrix!

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Example

Problem: `glasso` not robust!

Adding 10 outliers distributed according to $\mathbf{N}(\mathbf{10}, \mathbf{I}_3)$ leads to

```
> glasso(cov(X), rho=0.2)$wi
       [,1]   [,2]   [,3]
[1,]  0.504 -0.224 -0.283
[2,] -0.224  0.504 -0.216
[3,] -0.283 -0.216  0.552
```

Idea: Combine regularization of `glasso` with robust techniques!

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Regularized MCD estimator

Croux and Haesbroeck (2010):

Improvement: Adapt MCD idea and integrate it into log-likelihood function:

$$\mathcal{L}(H, (\boldsymbol{\mu}, \boldsymbol{\Theta})) = \log(\det(\boldsymbol{\Theta})) - \frac{1}{h} \sum_{i \in H} (\boldsymbol{x}_i - \boldsymbol{\mu})^\top \boldsymbol{\Theta} (\boldsymbol{x}_i - \boldsymbol{\mu}) - \lambda \|\boldsymbol{\Theta}\|_1$$

with

$$H \subseteq \{1, \ldots, n\}, \ |H| = h < n$$

Maximization of $\mathcal{L}(H, (\boldsymbol{\mu}, \boldsymbol{\Theta}))$ means to find an index subset H_{opt} for which

$$\max_{(\boldsymbol{\mu}, \boldsymbol{\Theta})} \mathcal{L}(H_{opt}, (\boldsymbol{\mu}, \boldsymbol{\Theta})) \geq \max_{(\boldsymbol{\mu}, \boldsymbol{\Theta})} \mathcal{L}(H, (\boldsymbol{\mu}, \boldsymbol{\Theta}))$$

$$\forall H \subseteq \{1, \ldots, n\} : |H| = h$$

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Regularized MCD estimator

Problem: $\binom{n}{h}$ subsets to check. Not applicable to large n.

Improvement: C-Step Algorithm: Let H_k be the subset derived at iteration k and $(\hat{\boldsymbol{\mu}}_{H_k}, \hat{\boldsymbol{\Theta}}_{H_k})$ be the corresponding estimates maximizing $\mathcal{L}(H_k, (\boldsymbol{\mu}, \boldsymbol{\Theta}))$.

Compute Mahalanobis distances with respect to $(\hat{\boldsymbol{\mu}}_{H_k}, \hat{\boldsymbol{\Theta}}_{H_k})$:

$$d_i^{(k)}(\boldsymbol{x}_i, \hat{\boldsymbol{\mu}}_{H_k}, \hat{\boldsymbol{\Theta}}_{H_k}) = \sqrt{(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_{H_k})^\top \hat{\boldsymbol{\Theta}}_{H_k} (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_{H_k})}$$

Define next subset H_{k+1} as

$$H_{k+1} = \left\{ i \in \{1, \ldots, n\} : d_i^{(k)} \in \{d_{(1)}^{(k)}, \ldots, d_{(h)}^{(k)}\} \right\}$$

where $d_{(j)}^{(k)}$ are the ordered distances.

$$\Rightarrow \mathcal{L}(H_k, (\boldsymbol{\mu}_{H_k}, \boldsymbol{\Theta}_{H_k})) \leq \mathcal{L}(H_{k+1}, (\boldsymbol{\mu}_{H_{k+1}}, \boldsymbol{\Theta}_{H_{k+1}}))$$

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Algorithm

The regularized MCD estimator is computed using the following algorithm:

1. Draw **initial subset** H_0
2. Maximize **penalized likelihood function** (`glasso`) to obtain $(\hat{\boldsymbol{\mu}}_{H_0}, \hat{\boldsymbol{\Theta}}_{H_0})$
3. Compute **ordered Mahalanobis distances** w.r.t. $(\hat{\boldsymbol{\mu}}_{H_0}, \hat{\boldsymbol{\Theta}}_{H_0})$
4. Choose next subset containing h observations with **smallest distances**
5. Repeat steps 2-4 until convergence to obtain $(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Theta}})$

$\Rightarrow$ A local maximum of the likelihood value is reached. Algorithm can be repeated several times with different initial subsets.

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LDA and RegMCD

How to apply LDA with the regularized MCD estimator in the multi group setting:

$$\mathbf{X} = \{\mathbf{x}_{ij} : i = 1, \ldots, n_j; j = 1, \ldots, k\}$$

- Compute **robust location estimates** $\boldsymbol{t}_j$ for $j = 1, \ldots, k$
- Compute **centered observations** $\mathbf{Z} = \{\boldsymbol{z}_{ij}\}$ with $\boldsymbol{z}_{ij} = \boldsymbol{x}_{ij} - \boldsymbol{t}_j$
- Apply the **regularized MCD algorithm** to $\mathbf{Z}$ to obtain common estimates $(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Theta}})$
- Correct location estimates: $\hat{\boldsymbol{\mu}}_j = \boldsymbol{t}_j + \hat{\boldsymbol{\mu}}$
- Apply LDA using parameters $\hat{\boldsymbol{\mu}}_1, \ldots, \hat{\boldsymbol{\mu}}_k, \hat{\boldsymbol{\Theta}}$

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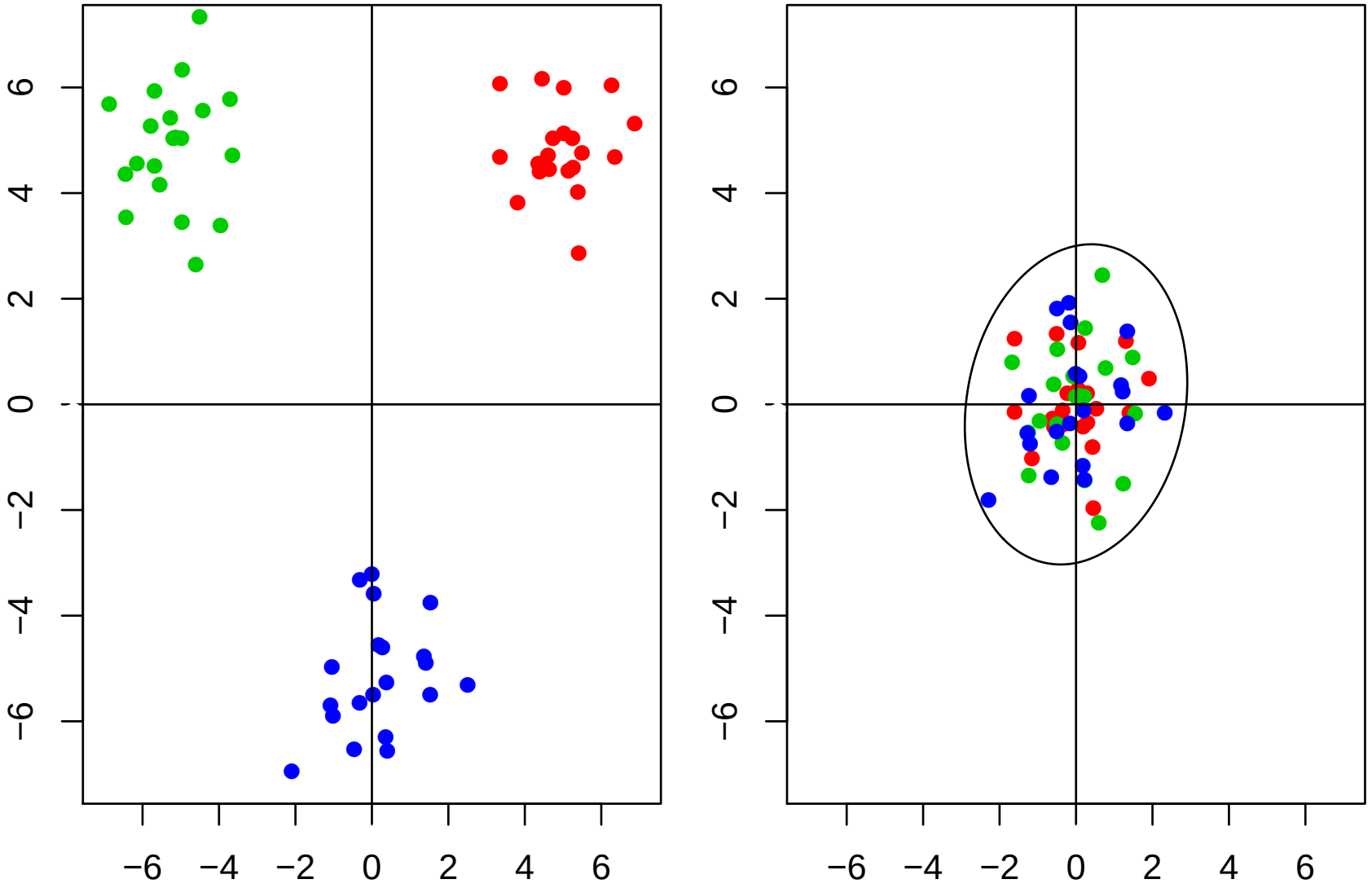
Centering



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The penalty parameter λ

How to choose the penalty parameter λ:

- Based on test error rates: Cross Validation
- Based on a model selection criterion: AIC, BIC

BIC criterion:

$$BIC(\Gamma) = -2 \cdot \log L(\Gamma) + \kappa(\Gamma) \log n$$

$L(\Gamma)$ . . . Likelihood function of the model
$\kappa(\Gamma)$ . . . Number of parameters in the model

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The penalty parameter λ

$BIC(\lambda)$ is small if

- the value of the likelihood function $\mathcal{L}(H_{opt}, \hat{\boldsymbol{\theta}})$ is high
- the number of parameters in the model is small

$\Rightarrow$ Choose λ according to

$$\lambda_{opt} = \arg\min_{\lambda} BIC(\lambda)$$

Best compromise between likelihood and sparseness!

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Example: Fruit Data

- Three different sorts of the same fruit (cucumis melo)
- 256 different spectra measured
- Outliers due to different illumination systems
- Partition of data into 60% training and 40% test set
- Test errors measured for each group separately

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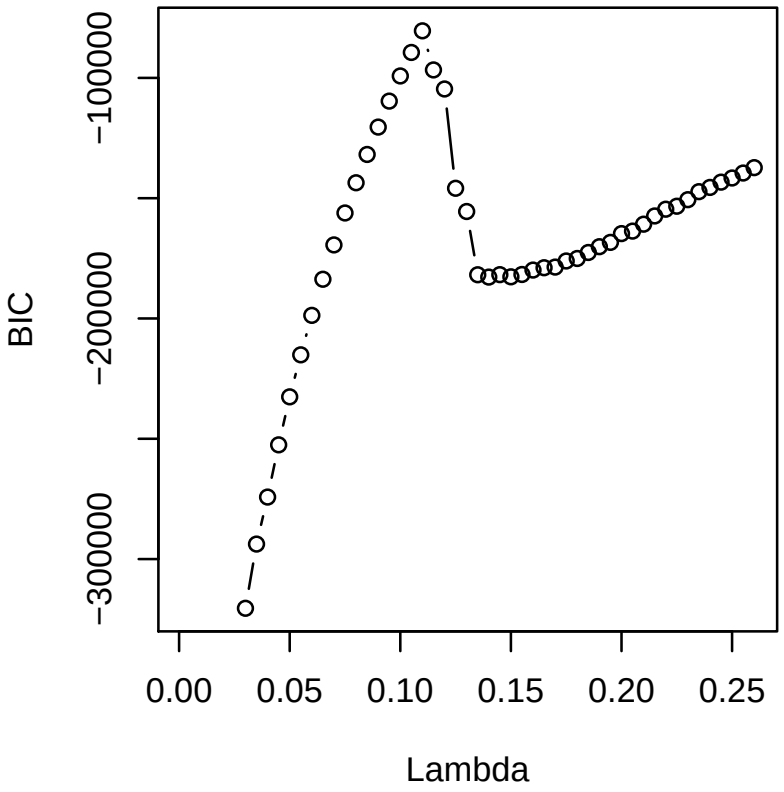
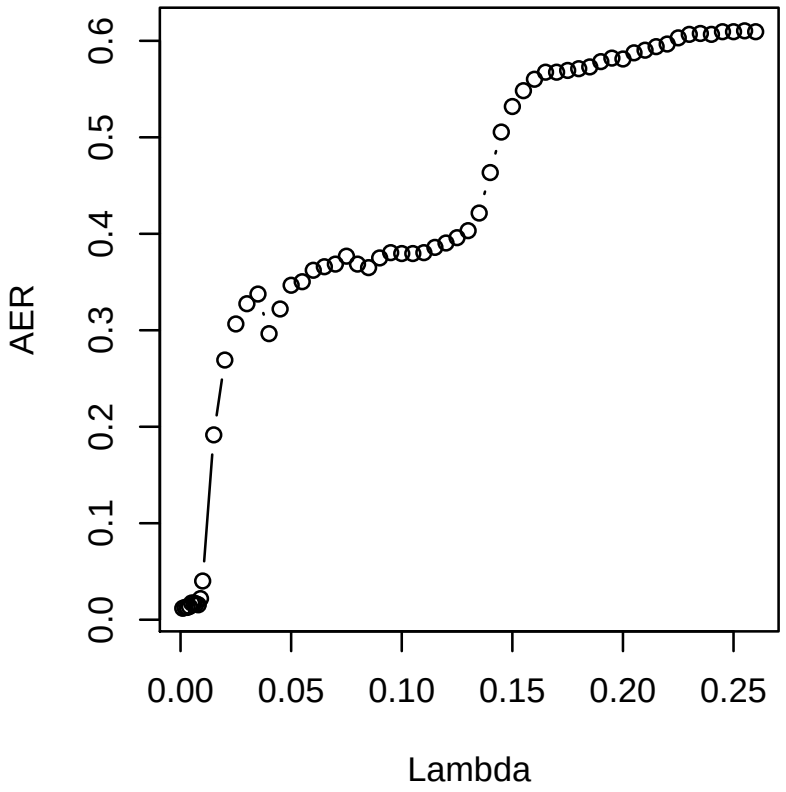
Example: Fruit Data, BIC

BIC and **AER** suggest a small λ value!





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Example: Fruit Data, Results

- **Outliers** in the third group lead to poor results for LDA.
- **RRLDA** remains stable!

	Err_{Test_1}	Err_{Test_2}	Err_{Test_3}
RRLDA ($\lambda = 0.001$)	0.02	0.03	0.01
GLASSO ($\lambda = 0.001$)	0.04	0.03	0.03
LDA	0.01	0.01	0.14

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Example: Golub Data, Results

- 38 training samples and 34 test samples from two cancer classes.
- Absolute test errors were measured for various variable subsets.
- Variable selection was done according to the nearest shrunken centroids method.

p	LDA	GLASSO	RRLDA
41	7	3	3
86	8	3	1
111	6	2	1
142	4	2	1
174	5	2	2
221	6	2	2
290	4	3	1
392	5	2	2
476	5	3	1
625	7	4	2

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Simulated Example

- Two groups ($k = 2$) both consisting of 100 observations and p variables with

$$p \in \{30, 100, 300, 500, 1000\}$$

- Discrimination occurs in variables 1 and 2.

- Variables 3 - p are uncorrelated noise according to standard normal distributions.

$$\boldsymbol{\mu}_1 = \begin{pmatrix} 0 \\ 1.9 \end{pmatrix} \quad \boldsymbol{\mu}_2 = \begin{pmatrix} 0 \\ -1.9 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0.7 \\ 0.7 & 1 \end{pmatrix}$$

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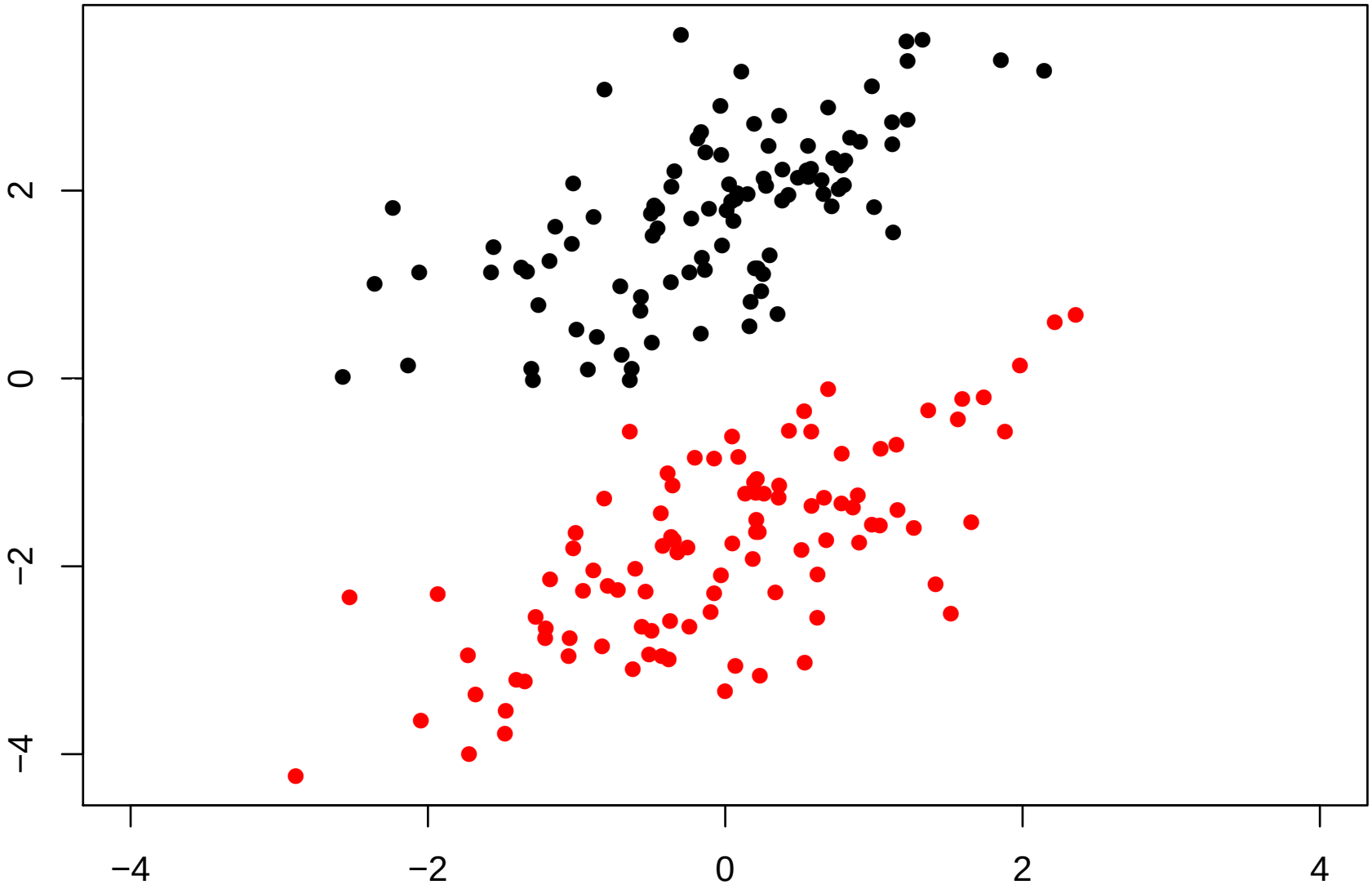
Simulated Example



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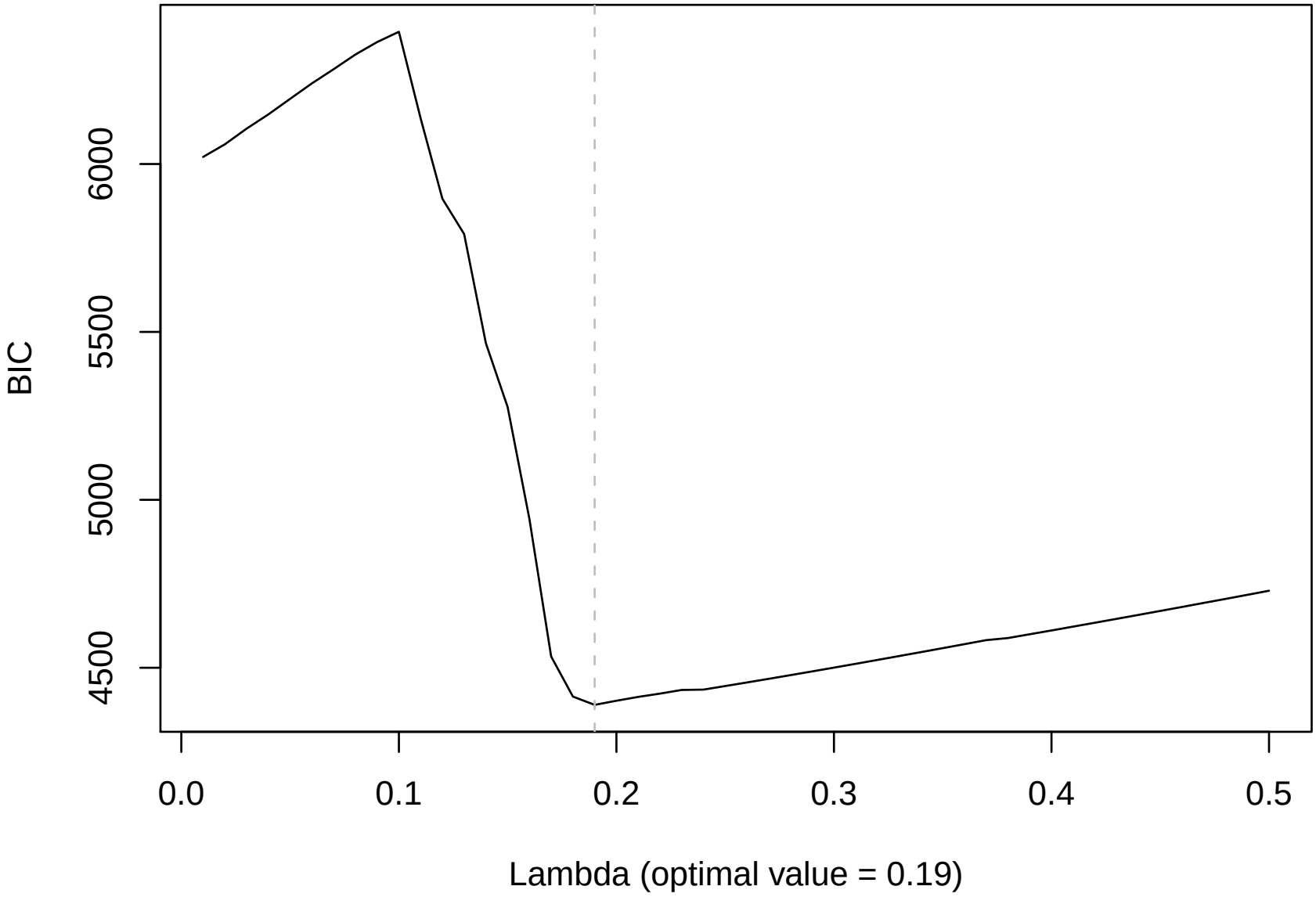
Simulated Example, BIC, p=30



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Simulated Example, Outliers

Simulate **contamination** by adding 10% **shift outliers** to the data.

- Variables 3 - p are distributed like non-outliers.
- Mean of variable 1 is shifted.
- Means of variable 2 are swapped.

$$\tilde{\mu}_1 = \begin{pmatrix} 10 \\ -1.9 \end{pmatrix} \quad \tilde{\mu}_2 = \begin{pmatrix} 10 \\ 1.9 \end{pmatrix}$$

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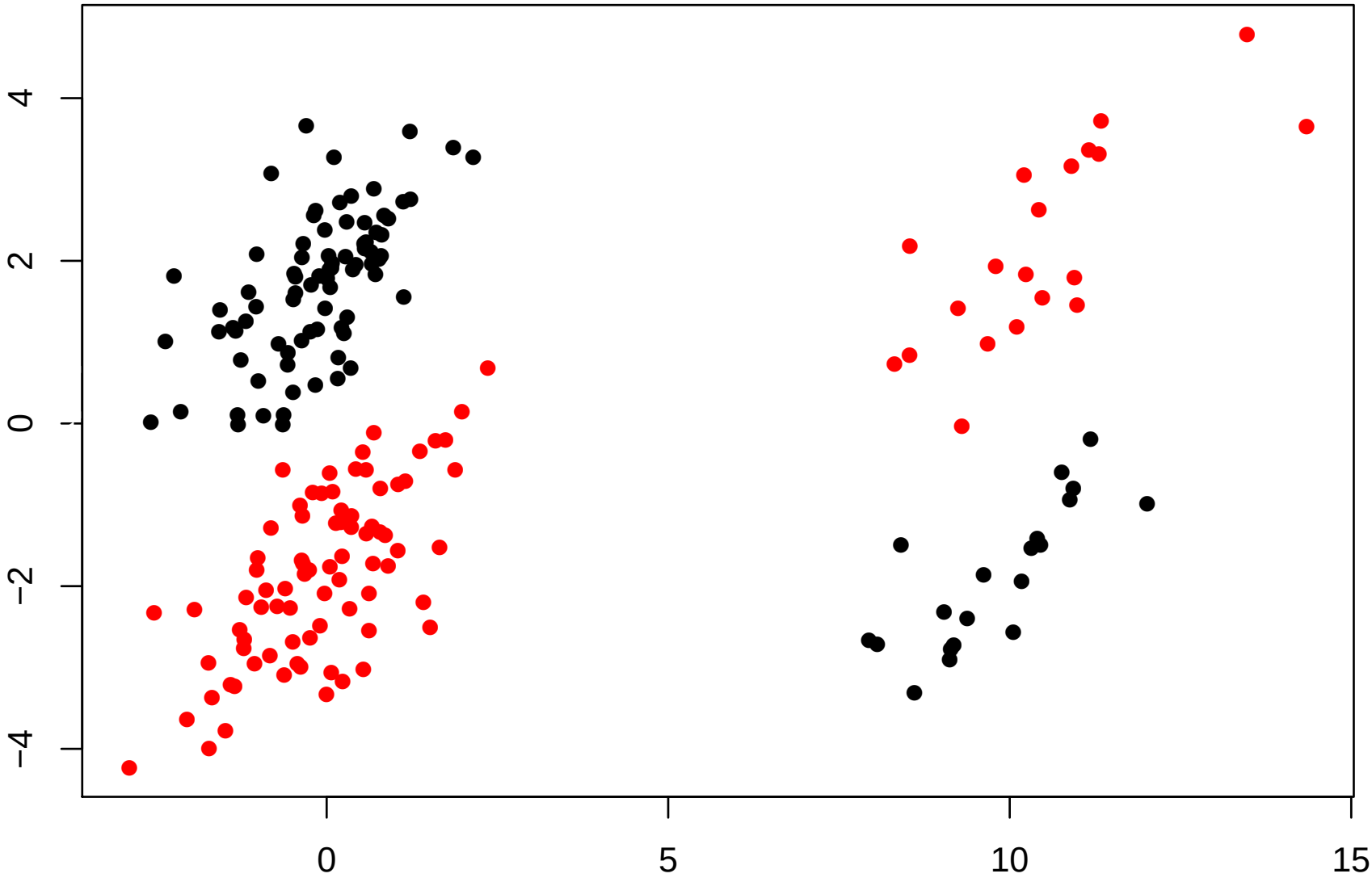
Simulated Example, Outliers



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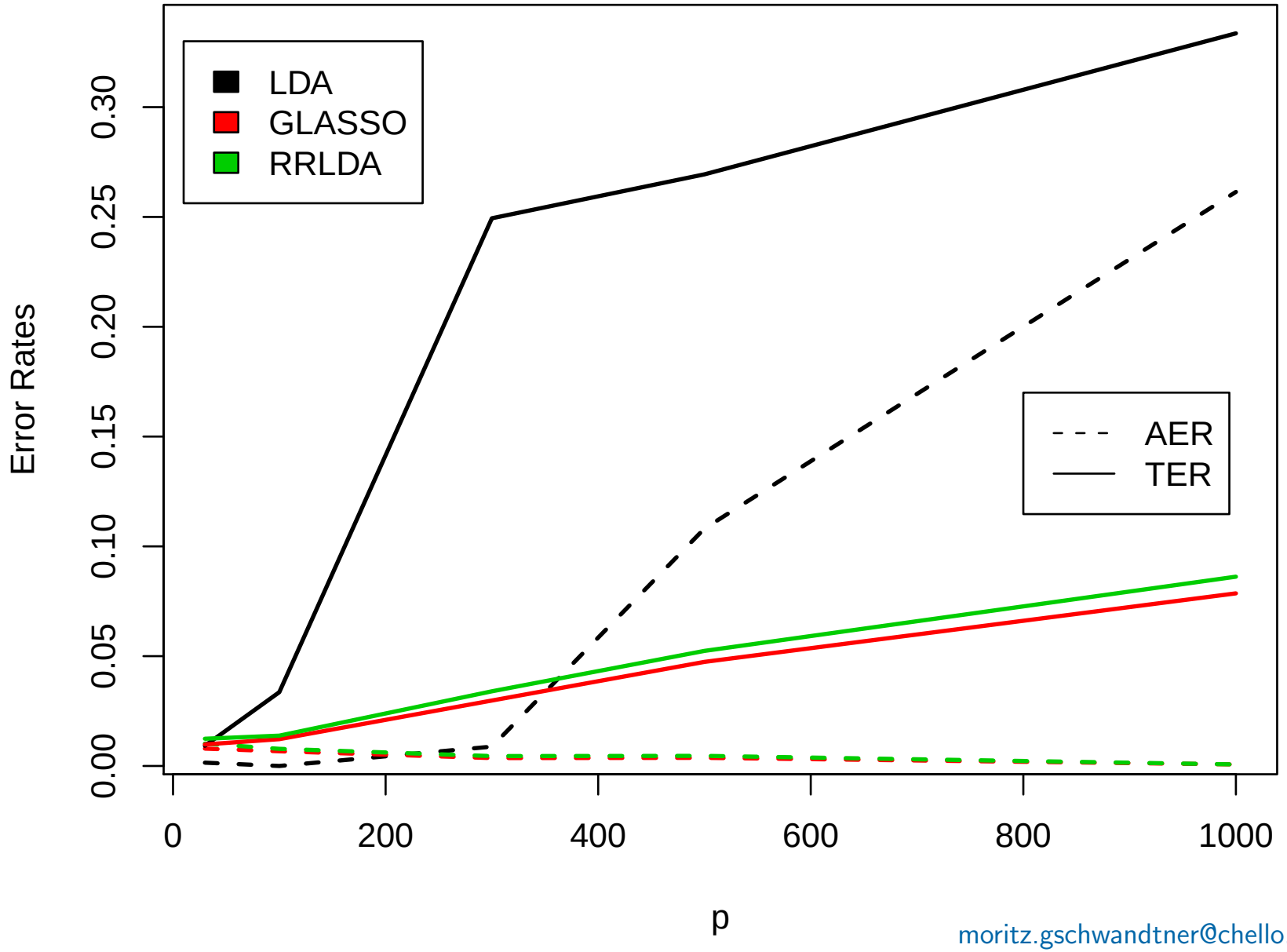
Results without contamination



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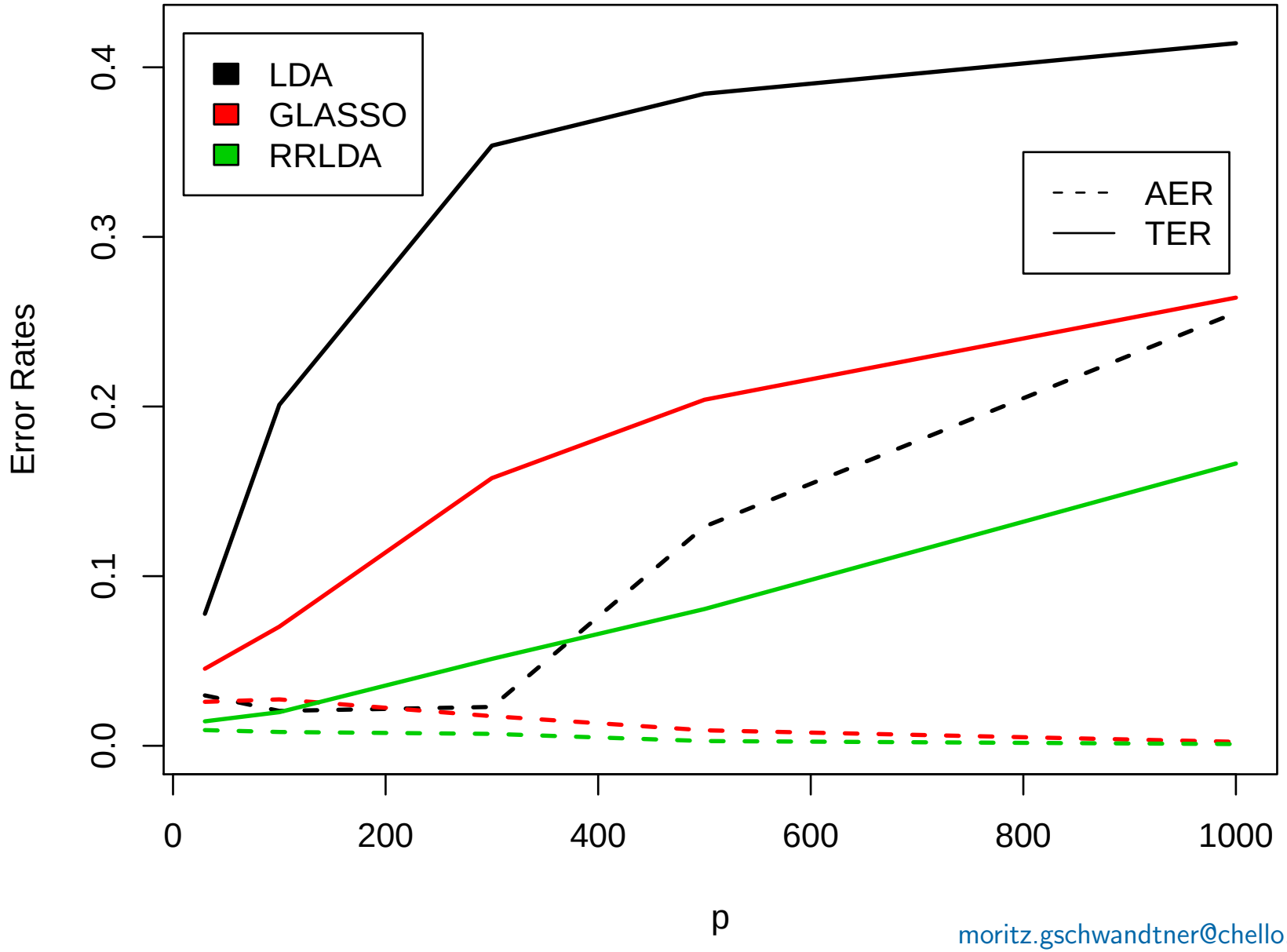
Results with contamination



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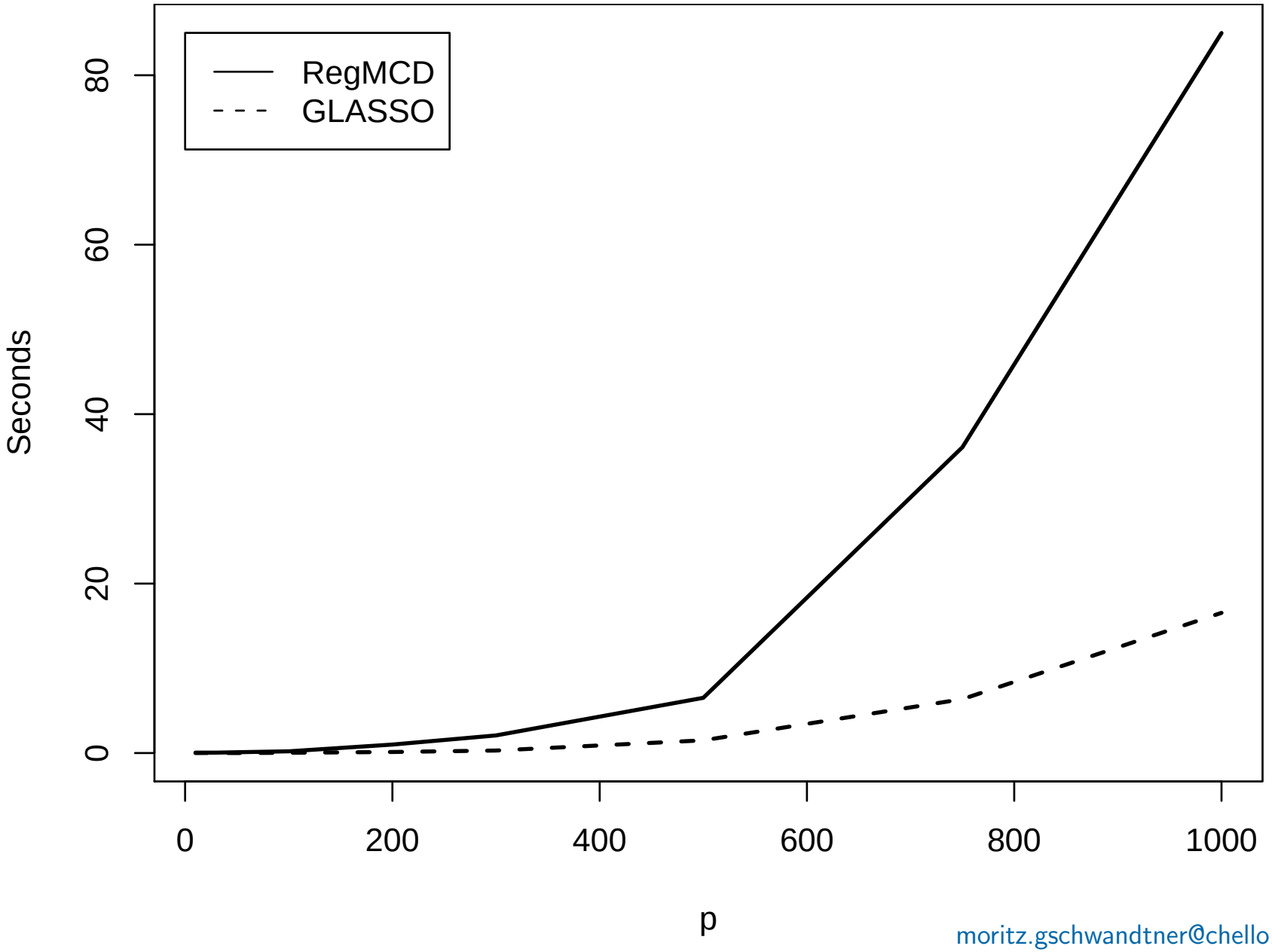
Computation Times



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Conclusions

- RRLDA is a combination of **regularization** and **robust methods**.
- RRLDA is a good choice if data contain either **outliers** or many **noisy variables** or both.
- Penalty parameter λ is chosen according to an **adapted BIC criterion**.

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Some references

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