Multivariate Regression und Klassifikation mit Anwendungen aus der Chemometrie

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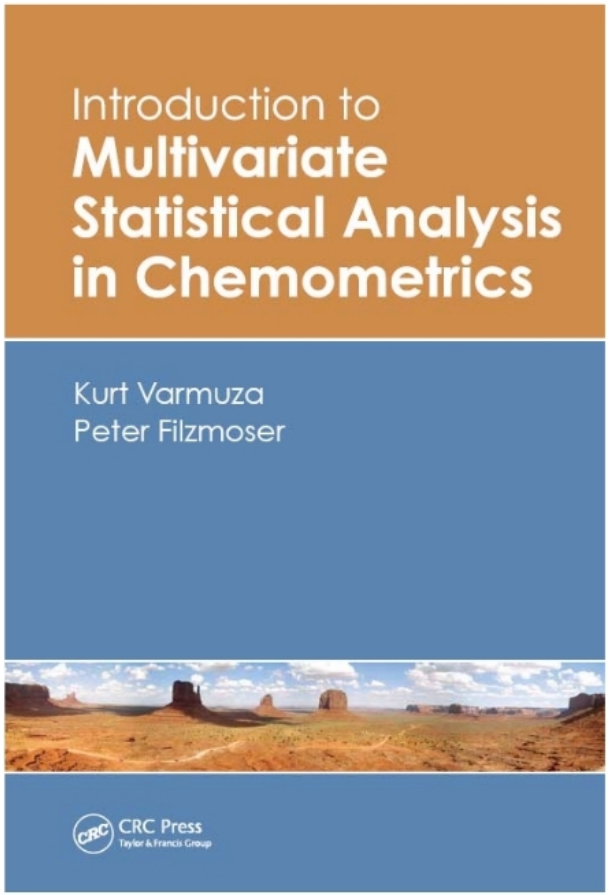
Overview

321 + xiii pages; around 100 figures; appeared in 2009.

Written by a **chemometrician** and a **statistician**, reflects both the **practical** approach to chemometrics and the more **formally oriented** one of statistics.



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Regression in high dimension

Consider the **multiple linear regression model**

$$y_i = \boldsymbol{x}_i^\top \boldsymbol{\beta} + \varepsilon_i \quad \text{for } i = 1, \ldots, n,$$

with
$\boldsymbol{y} = (y_1, \ldots, y_n)^\top$
$\boldsymbol{x}_i^\top = (1, x_{i1}, \ldots, x_{ip})$, forming the rows of $\boldsymbol{X}$,
$\boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_p)^\top$.

The **ordinary least-squares solution**

$$\hat{\boldsymbol{\beta}}_{\text{OLS}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

cannot be computed if $\boldsymbol{X}^\top \boldsymbol{X}$ is (near) singular. This happens typically in case of **multicollinearity or** $n < p$.

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Principal Component Regression (PCR)

Way out: Dimension reduction in the $\boldsymbol{X}$ space.

Assume that the $n \times p$ matrix $\boldsymbol{X}$ is mean-centered.
Representation with the first k **principal components (PCs)**:

$$\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{V}^\top + \boldsymbol{E}$$

with $\boldsymbol{Z}$ the $n \times k$ matrix of the first k PCs
$\boldsymbol{V}$ the $p \times k$ matrix with the first k PC loadings
$\boldsymbol{E}$ the error matrix ("reconstruction error")

Principal Component Regression:

$$\boldsymbol{y} = \boldsymbol{Z}\boldsymbol{\theta} + \varepsilon$$

with new regression coefficients $\boldsymbol{\theta}$ and errors ε.

Important: "tuning" parameter k

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Principal Component Regression (PCR)

PCR is a “technical” solution to the problem of multicollinearity:

- The PCs $\boldsymbol{Z}$ contain the “most important” information of $\boldsymbol{X}$. But is this also the most important part for explaining $\boldsymbol{y}$?
- Why take the first k PCs, and not a “variable selection” of PCs?
- The real problem is to find that information of $\boldsymbol{X}$ that is best suited for explaining $\boldsymbol{y}$.

Solution: Partial Least Squares (PLS) regression

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Partial Least Squares (PLS) regression

Use again a **"latent variable model"** to explain $\boldsymbol{X}$:

$$\boldsymbol{X} = \boldsymbol{T}\boldsymbol{A}^\top + \boldsymbol{E}$$

with *scores* $\boldsymbol{T}$ $(n \times k)$
and *loadings* $\boldsymbol{A}$ $(p \times k)$

The columns of $\boldsymbol{A}$ are derived by

$$\boldsymbol{a}_j = \underset{\boldsymbol{a}}{\text{argmax}}\, \text{Cov}(\boldsymbol{y}, \boldsymbol{X}\boldsymbol{a})$$

$(j = 1, \ldots, k)$.
Then we have the **new regression model**:

$$\boldsymbol{y} = \boldsymbol{T}\boldsymbol{\gamma} + \varepsilon = (\boldsymbol{X}\boldsymbol{A})\boldsymbol{\gamma} + \varepsilon$$

$$= \boldsymbol{X}\underbrace{(\boldsymbol{A}\boldsymbol{\gamma})}_{\boldsymbol{\beta}} + \varepsilon = \boldsymbol{X}\boldsymbol{\beta} + \varepsilon$$

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Partial Least Squares (PLS) regression

Important for PLS: selection of the "optimal" number k of PLS components.

- k too small: underfit; poor prediction ability of the model
- k too large: overfit, and again poor prediction ability of the model

Model evaluation requires **training**, **validation** and **test** data.

Since we have **only one data set** available, we have to split appropriately.

Performance measures for regression

Popular in chemometrics: **Standard Error of Prediction (SEP):**

$$\text{SEP} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(y_i - \hat{y}_i - \text{bias})^2}$$

with

$$\text{bias} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)$$

N is the number of test set observations.

Popular in many fields: **Mean Squared Error of Prediction (MSEP):**

$$\text{MSEP} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

We see that $\text{SEP}^2 = \text{MSEP} - \text{bias}^2$

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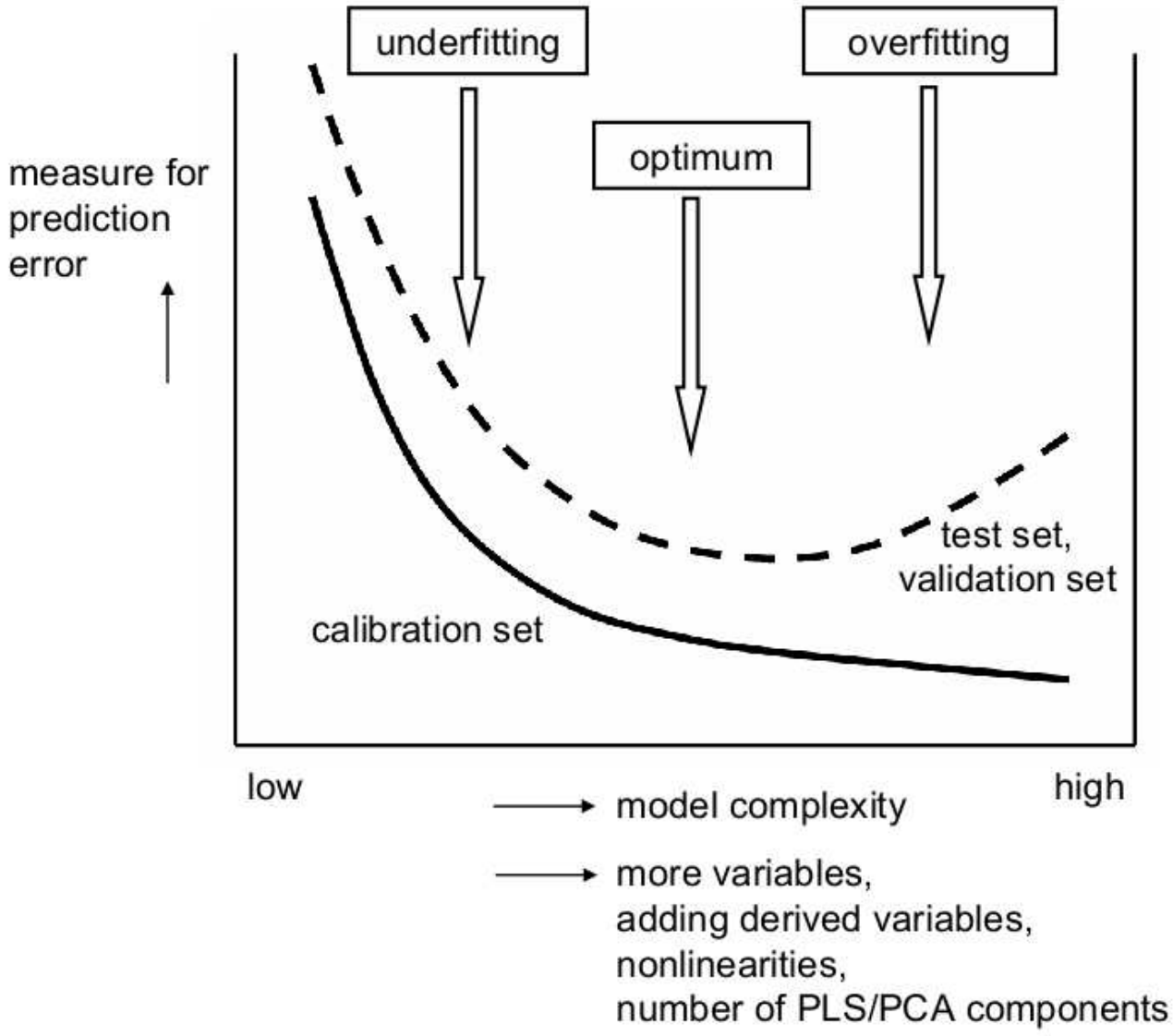
Optimal model complexity



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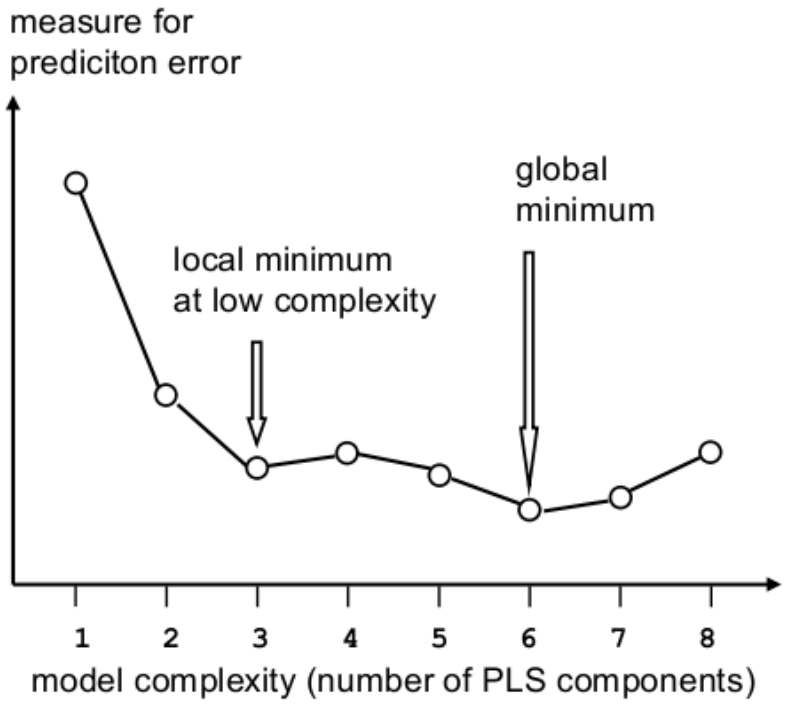
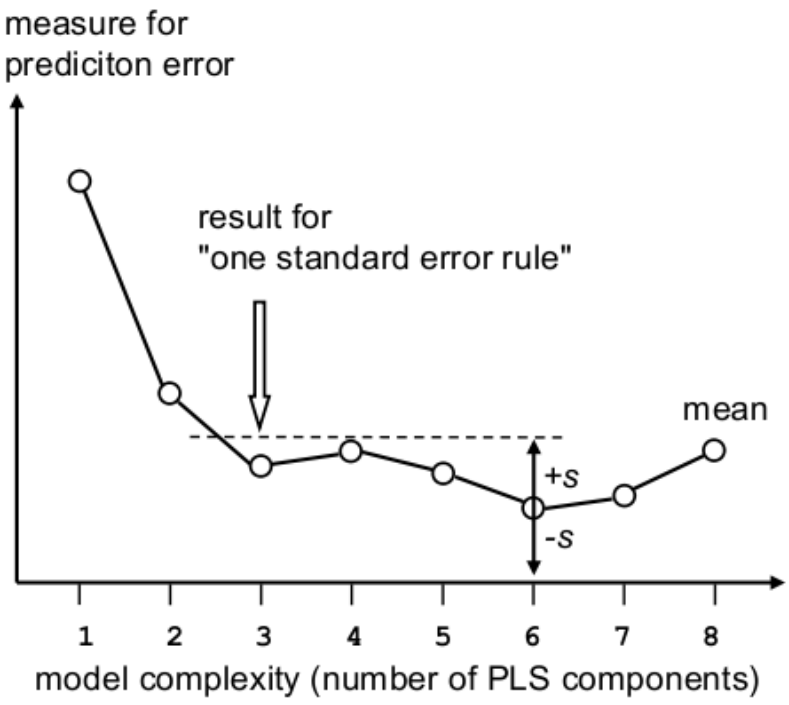
Optimal model complexity





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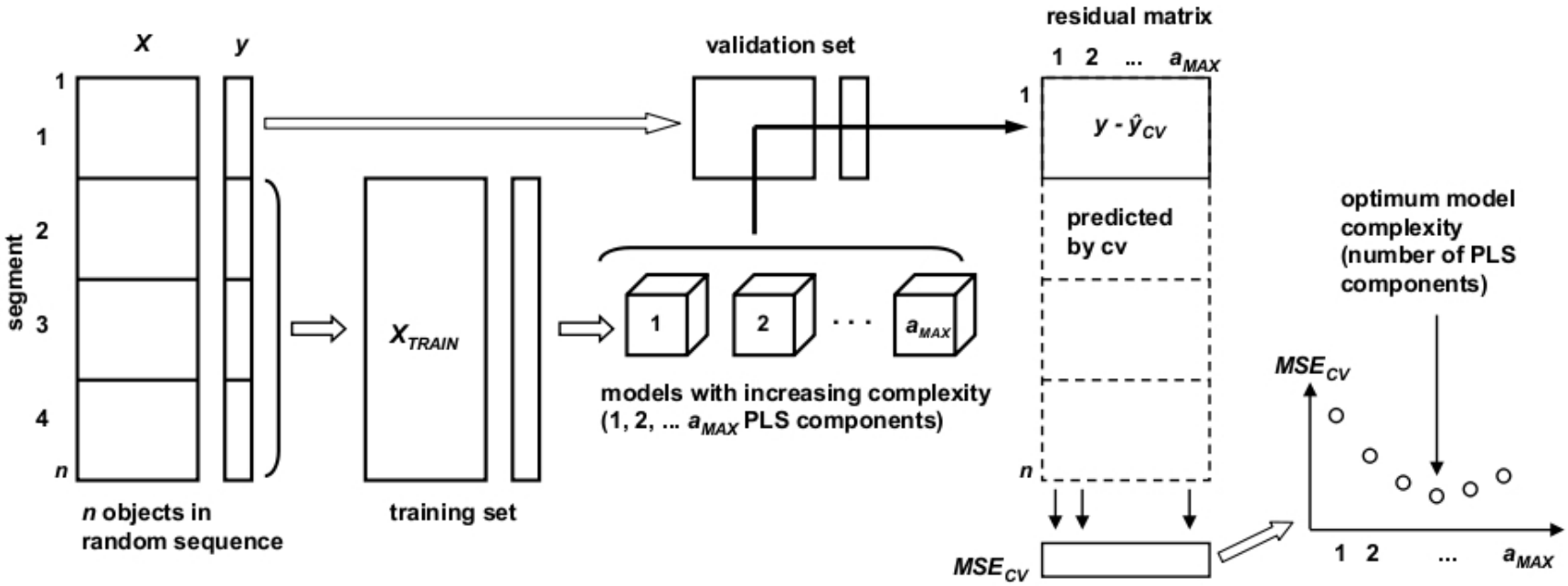
Cross Validation



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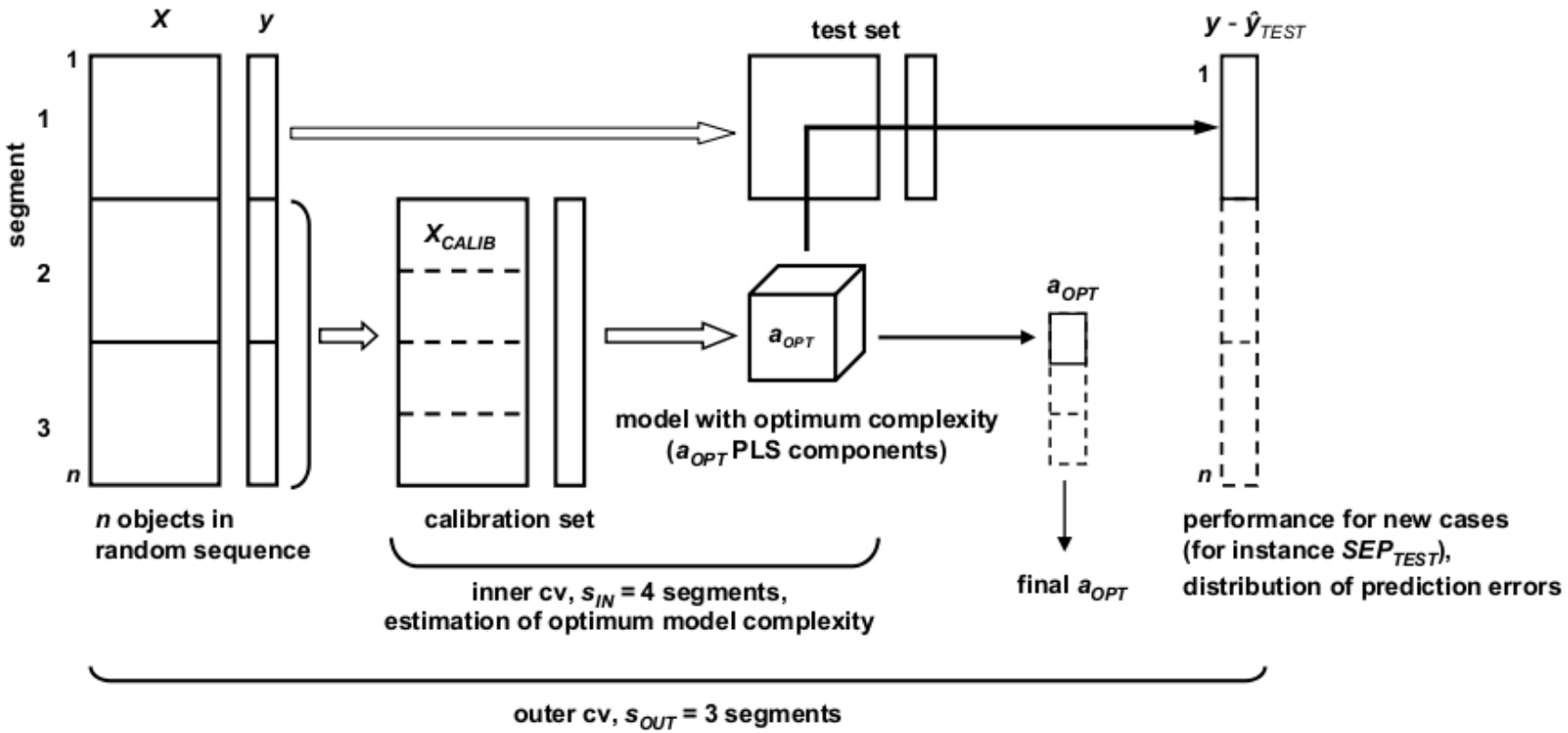
Repeated Double Cross Validation



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Regression & Shrinkage

Ridge regression (Hoerl and Kennard, 1970) is a solution to the problem of multicollinearity. The Ridge estimator is

$$\widehat{\boldsymbol{\beta}}_{\text{Ridge}} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

and it solves the problem

$$\widehat{\boldsymbol{\beta}}_{\text{Ridge}} = \underset{\boldsymbol{\beta}}{\text{argmin}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 \right\} \quad \text{with} \quad \sum_{j=1}^{p} \beta_j^2 \leq \text{const.}$$

The Ridge parameter λ **shrinks the regression coefficients** (regularization).

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Regression & Shrinkage

Lasso regression (Tibshirani, 1996) solves the problem

$$\hat{\boldsymbol{\beta}}_{\text{Lasso}} = \underset{\boldsymbol{\beta}}{\text{argmin}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 \right\} \quad \text{with} \quad \sum_{j=1}^{p} |\beta_j| \leq \text{const.}$$

No explicit formula for the solution, only numerical optimization.

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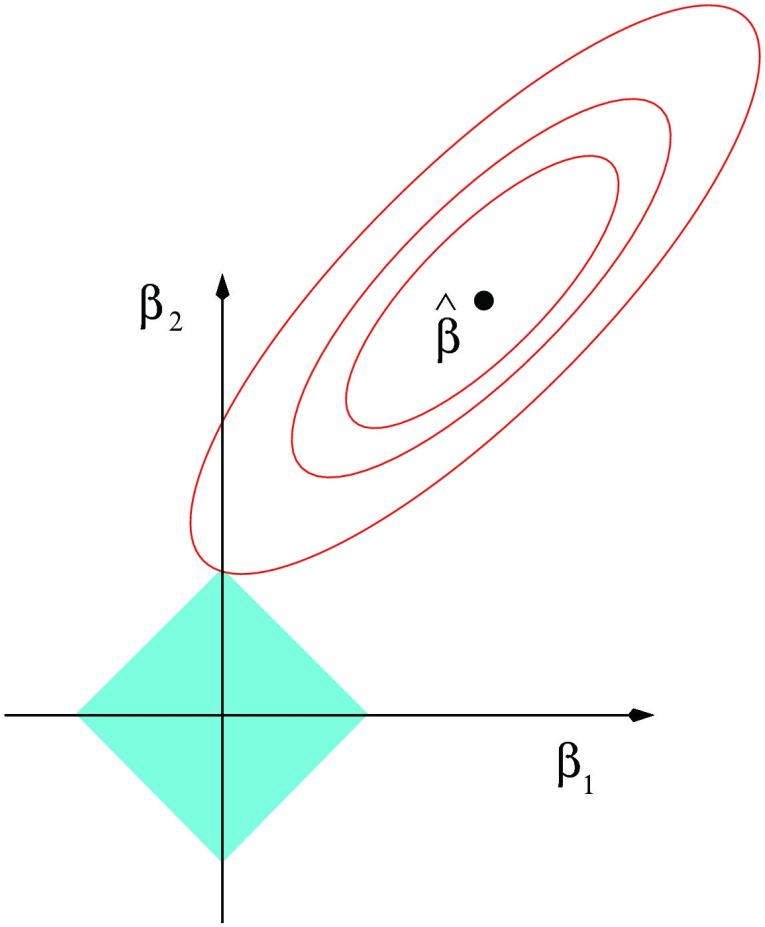
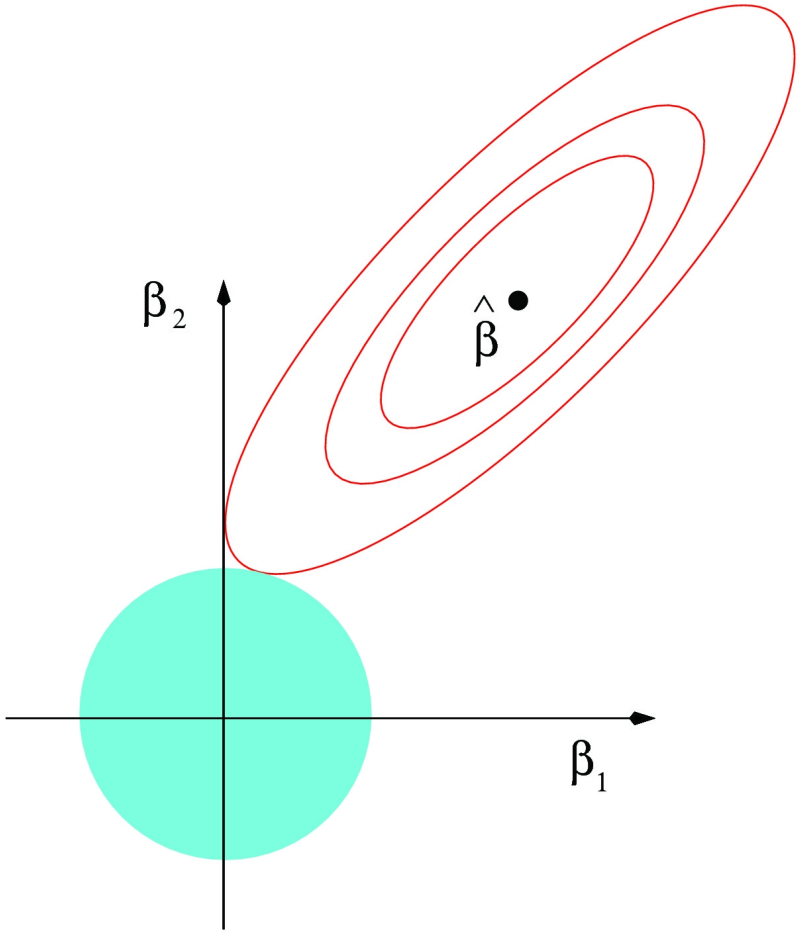
Lasso versus Ridge

Lasso: $\sum_{j=1}^{p} |\beta_j| \leq \text{const}$



Ridge: $\sum_{j=1}^{p} \beta_j^2 \leq \text{const}$



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Software in R: package “chemometrics”

Freely available in R: `http://www.r-project.org`

Main contributions of the “chemometrics” package:

- Robustness (e.g. robust PLS)
- Model evaluation (e.g. repeated double cross-validation)
- Unified evaluation tools for parameter selection
- Diagnostic tools (e.g. for choice of number of components, visualizing effect of outliers)
- Example data sets

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Multivariate Calibration

Example data:

Gas chromatographic retention indices of polycyclic aromatic compounds:

We consider $n = 209$ polycyclic aromatic compounds (PAC):

y-vector: GC retention index;

X-matrix: $p = 467$ descriptors of the molecular structure (Corina, Dragon).

```
> library(chemometrics)
> data(PAC)
> str(PAC)

List of 2
 $ y: num [1:209] 197 197 197 200 201 ...
 $ X: num [1:209, 1:467] 6.51 6.51 6.01 7.12 8.95 6.62 7.32 7.6 7.6 6.77 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:209] "1" "2" "3" "4" ...
  .. ..$ : chr [1:467] "AMW" "Me" "Mp" "Ms" ...
```

PLS (and PCR)

Idea: reduce the number of regressor variables to a few components (PCR: using only the X-data; PLS: using both X and y data).

```
> pls_dcv <- mvr_dcv(y~X,ncomp=50,data=PAC,method="simpls")
             # PLS with repeated double cross validation
             # Default: 100 repetitions, 4 outer and 10 inner segments
             # for PCR use: method="svdpc"
```

Output:

```
 $ resopt  : num [1:209, 1, 1:100]
 $ predopt : num [1:209, 1, 1:100]
 $ optcomp : int [1:4, 1:100]
 $ pred    : num [1:209, 1, 1:50, 1:100]
 $ SEPopt  : num 12
 $ sIQRopt : num 8.4
 $ sMADopt : num 8.39
 $ MSEPopt : num 144
 $ afinal  : num 11
 $ SEPfinal: Named num [1:50]
```

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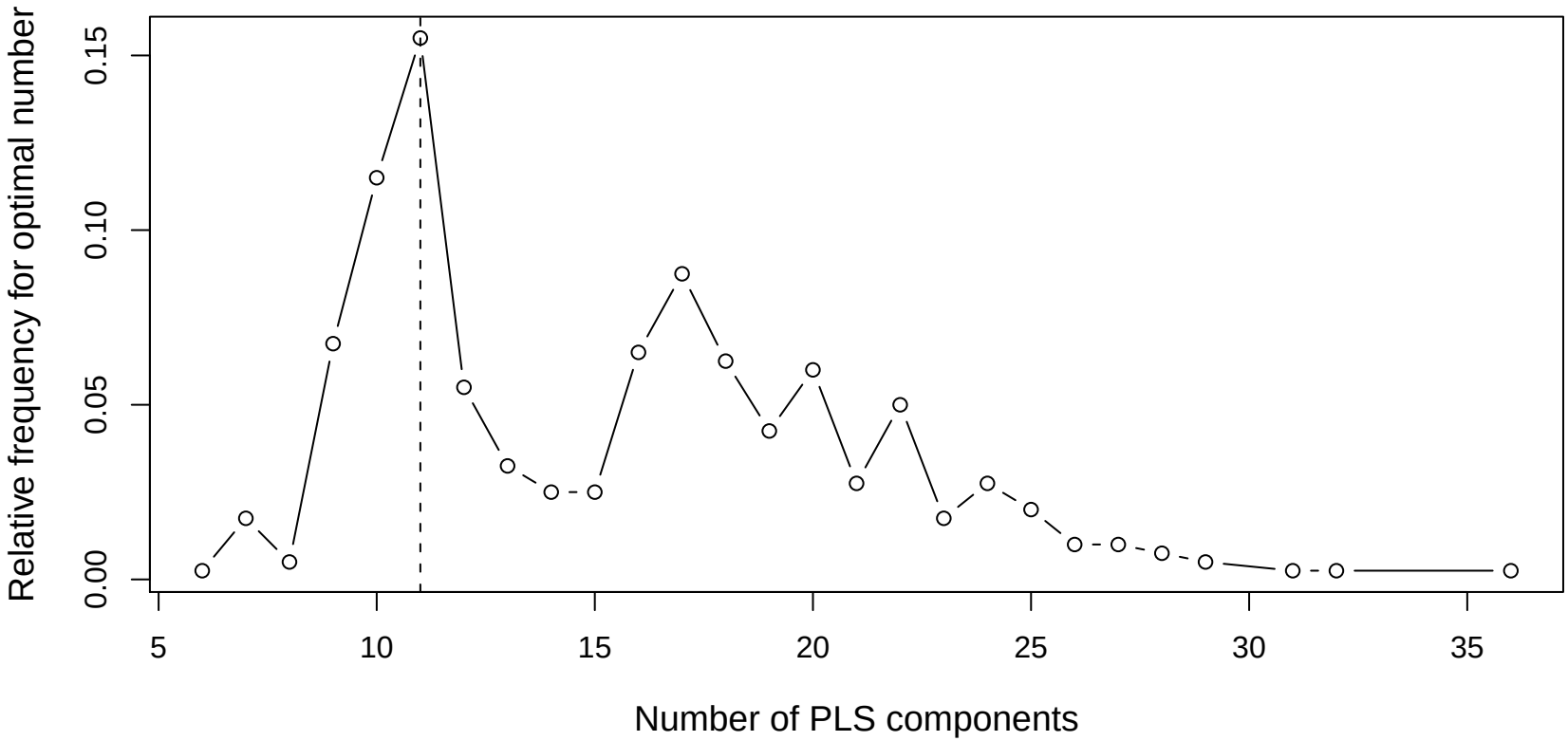
PLS (and PCR)

Diagnostic plots: optimal number of components (based on 4×100 values)

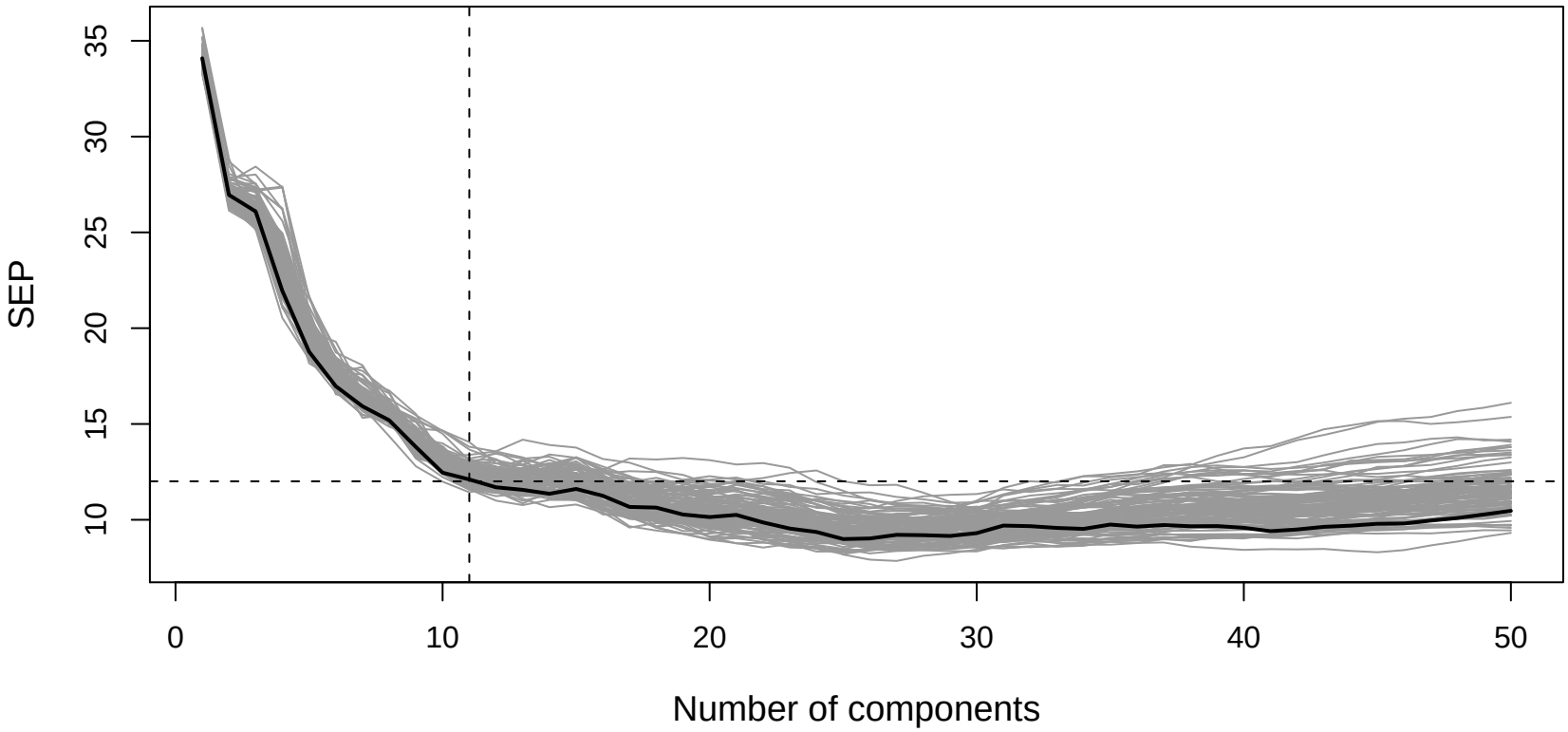
```
> plotcompmvr(pls_dcv)
```



PLS (and PCR)

Diagnostic plots: SEP for $1, \ldots, 50$ components

```
> plotSEPmvr(pls_dcv,optcomp=11,y=PAC$y,X=PAC$X,method="simpls")
```



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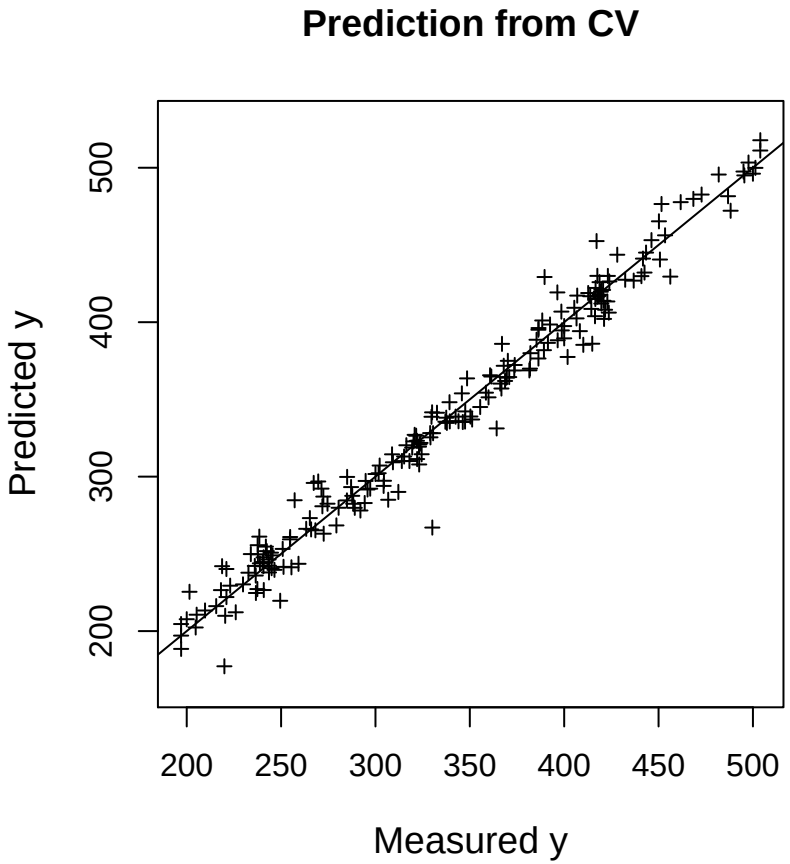
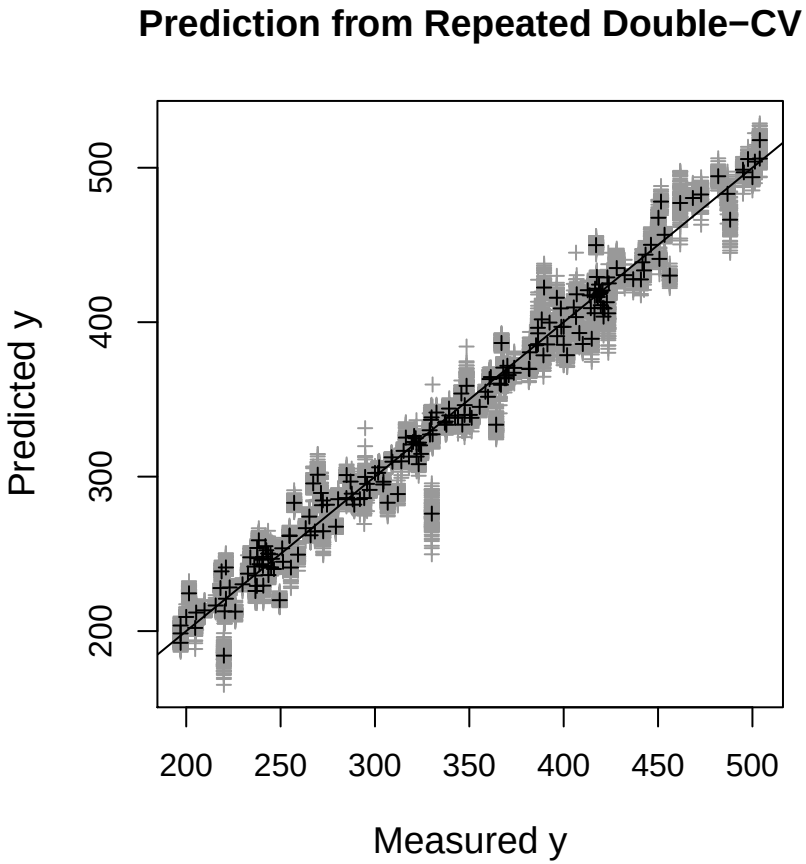
PLS (and PCR)

Diagnostic plots: predicted values from 100 models with 11 components

```
> plotpredmvr(pls_dcv,optcomp=11,y=PAC$y,X=PAC$X,method="simpls")
```





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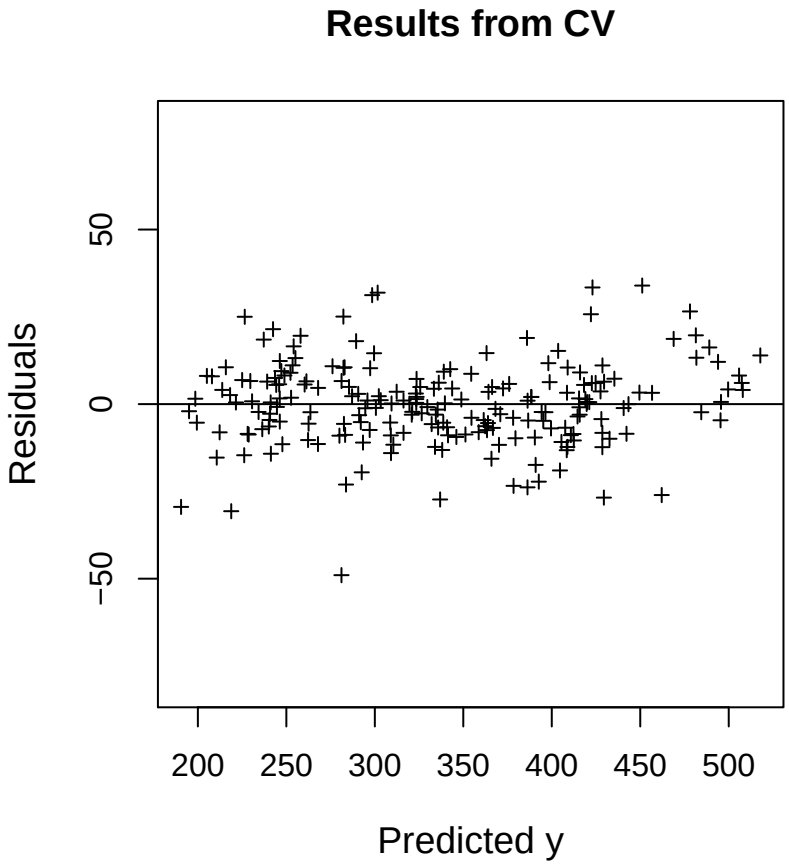
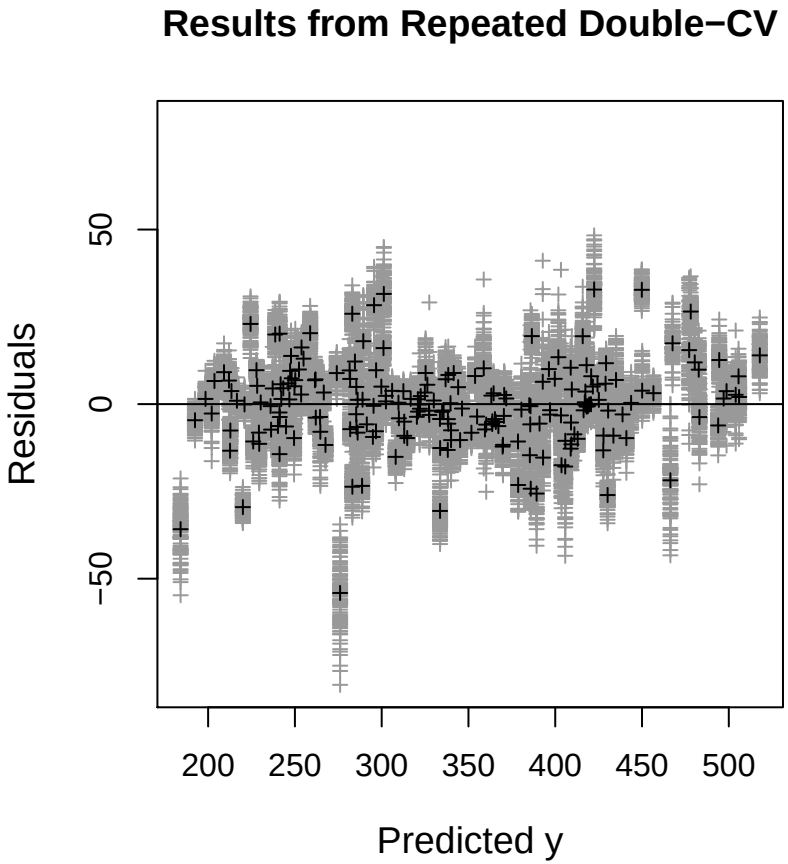
PLS (and PCR)

Diagnostic plots: residuals from 100 models with 11 components

```
> plotresmvr(pls_dcv,optcomp=11,y=PAC$y,X=PAC$X,method="simpls")
```





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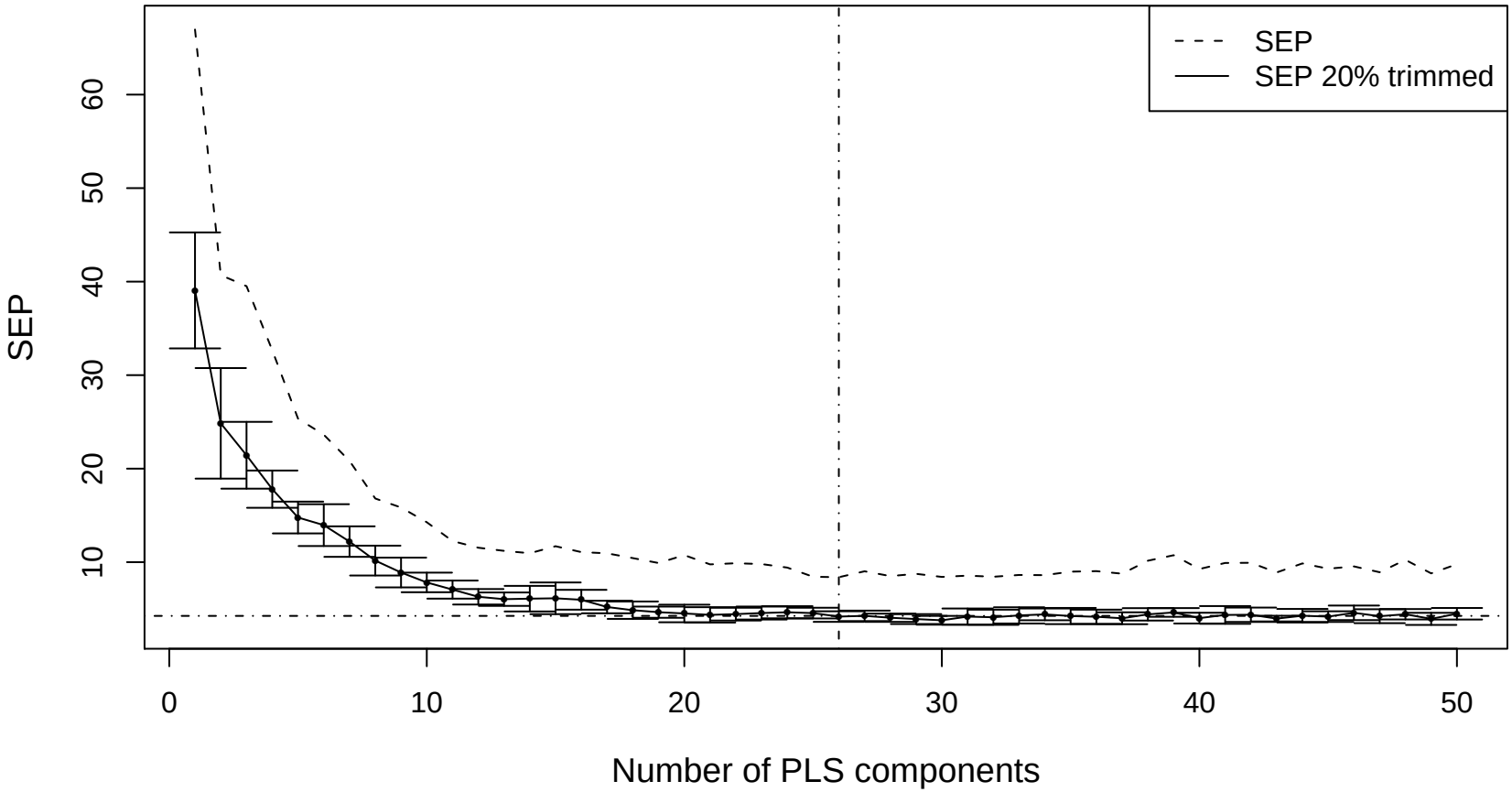
Robust PLS

PRM: Serneels, Croux, Filzmoser, Van Espen (ChemoLab, 2005)

```
> prm_cv(PAC$X,PAC$y,a=50,trim=0.2,plot.opt=TRUE)
```



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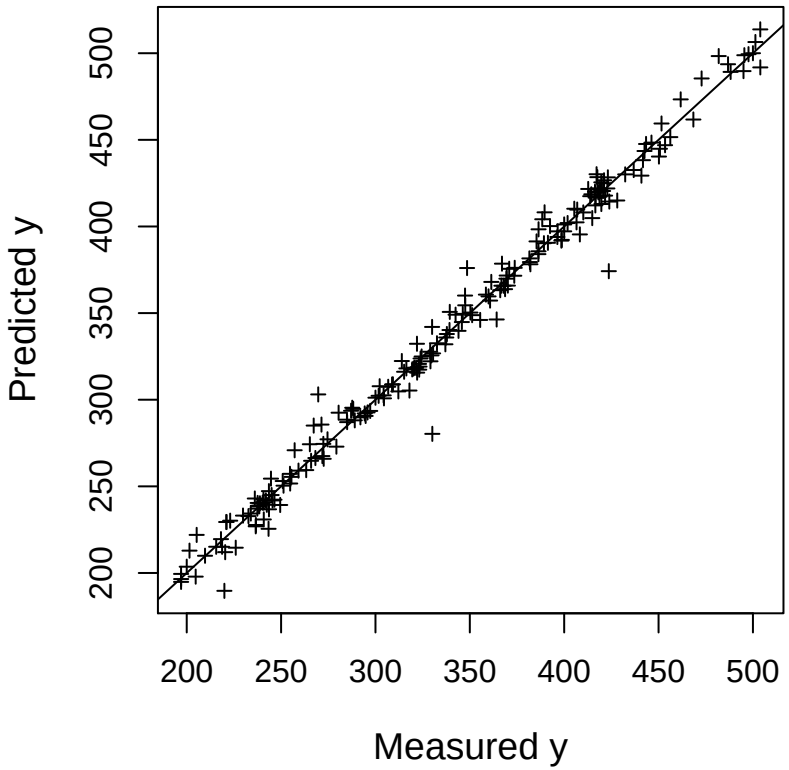
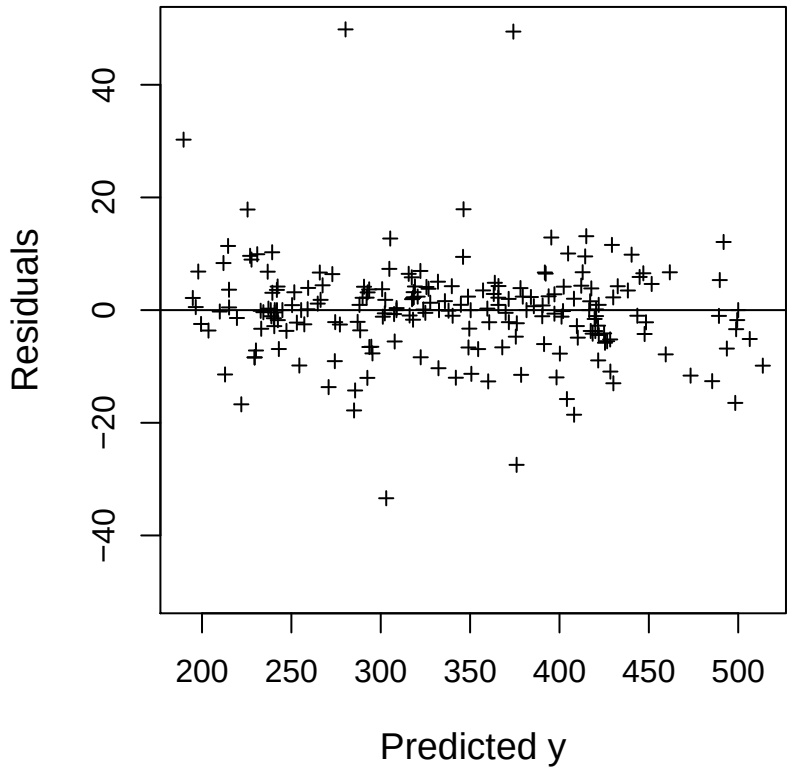
Robust PLS

Diagnostic plots: predicted values and residuals using 26 components

```
> plotprm(resprmcv,PAC$y)
```





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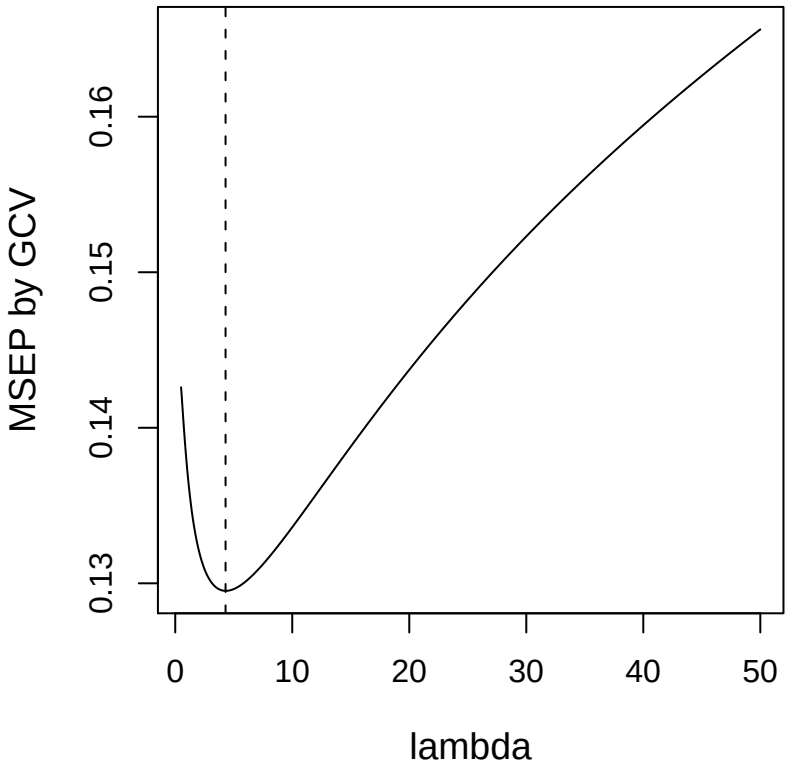
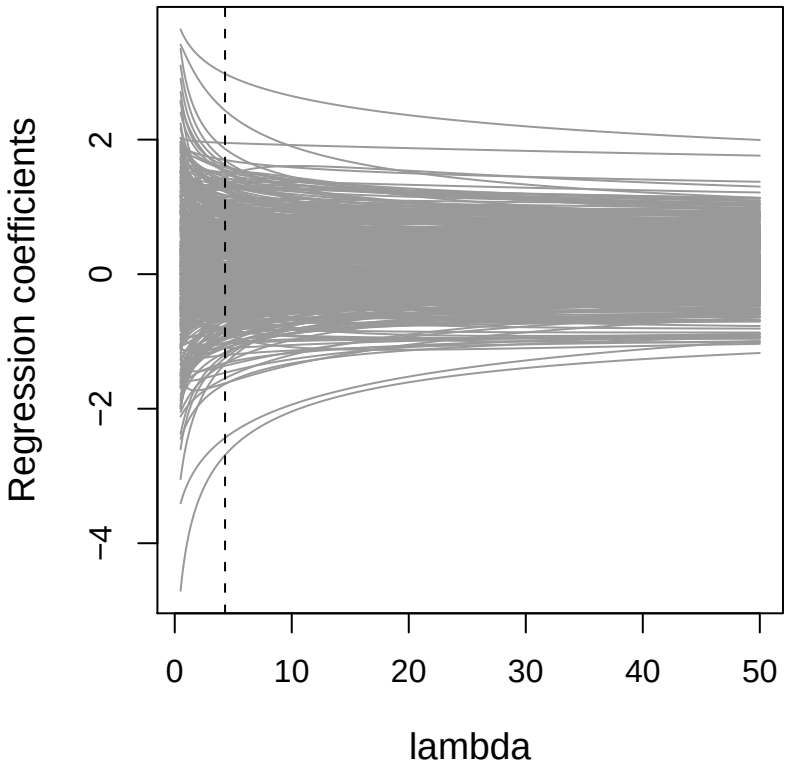
Ridge Regression

Diagnostic plot: choice of ridge parameter

```
> resR <- plotRidge(y~X,data=PAC,lambda=seq(0.5,50,by=0.05))
```





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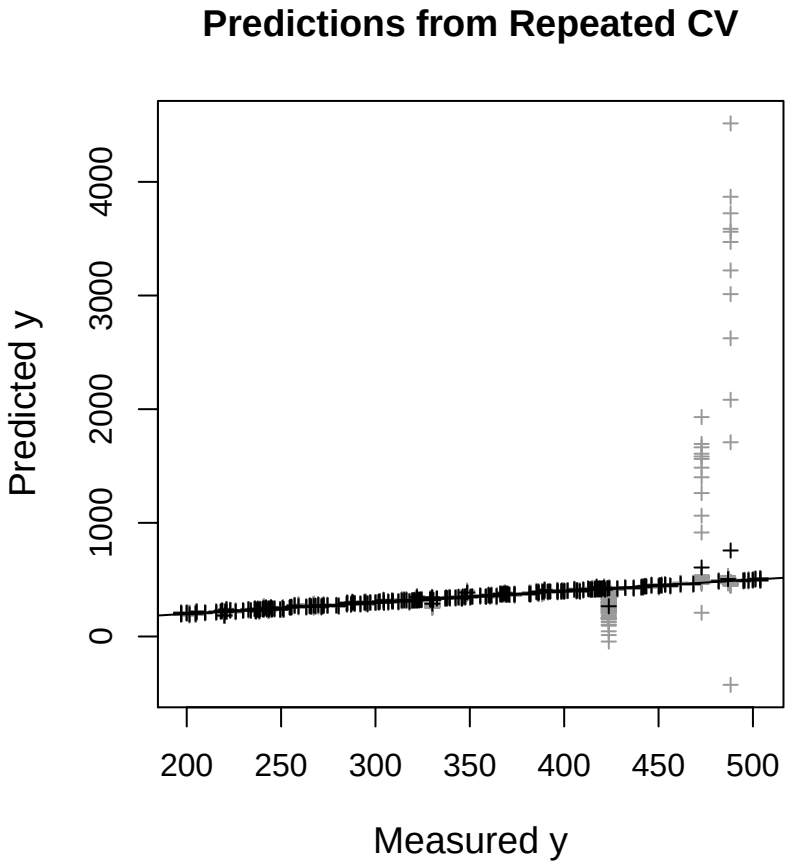
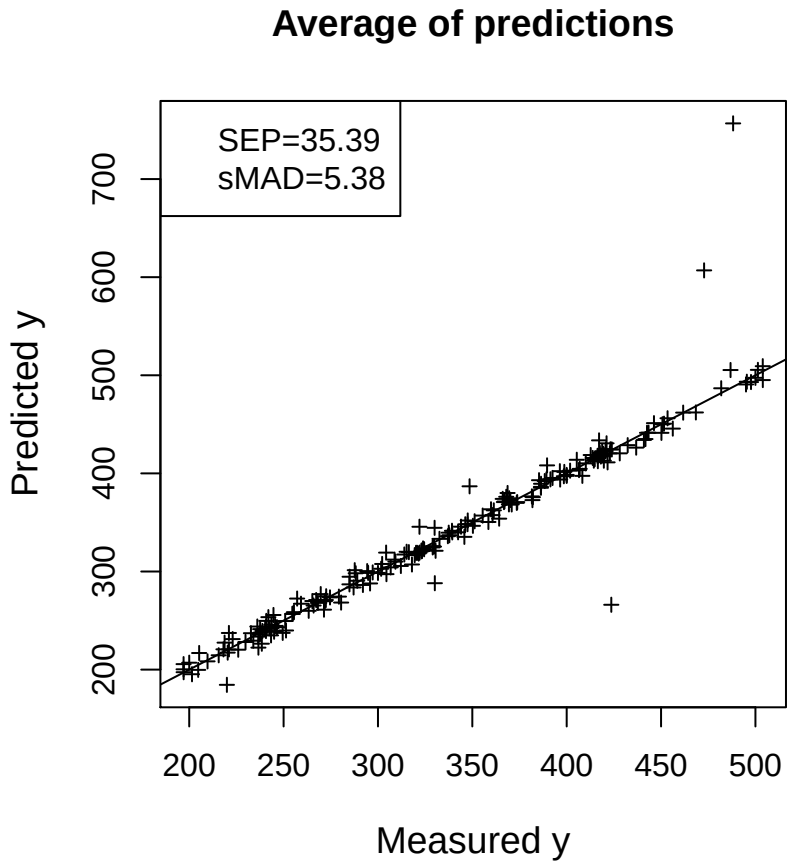
Ridge Regression

Diagnostic plots: from repeated cross validation

```
> resRcv <- ridgeCV(y~X,data=PAC,repl=100,lambda=resR$lambdaopt)
```





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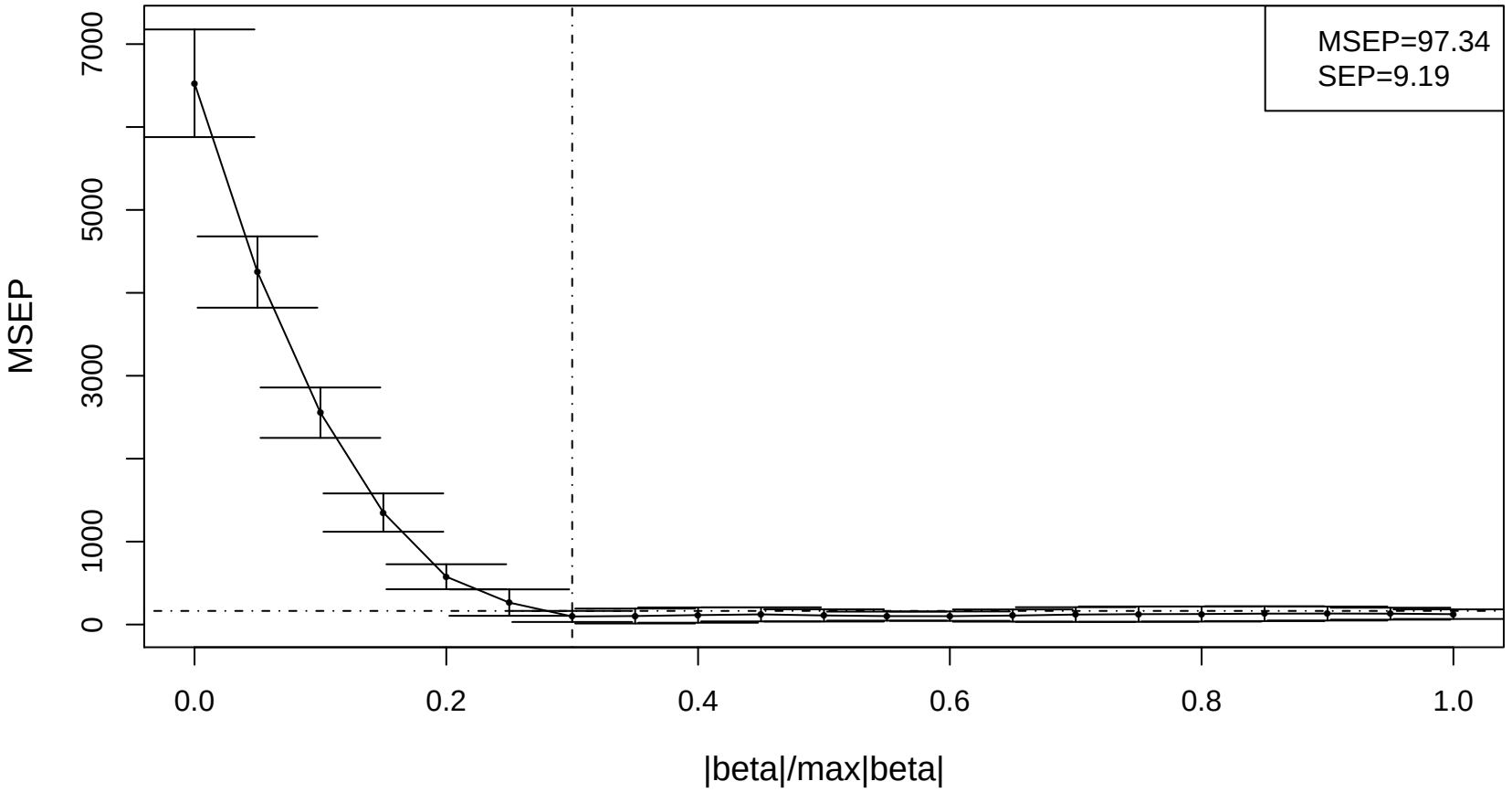
Lasso Regression

Diagnostic plot: choice of Lasso parameter

```
> resL <- lassoCV(y~X,data=PAC,K=10,fraction=seq(0,1,by=0.05))
```



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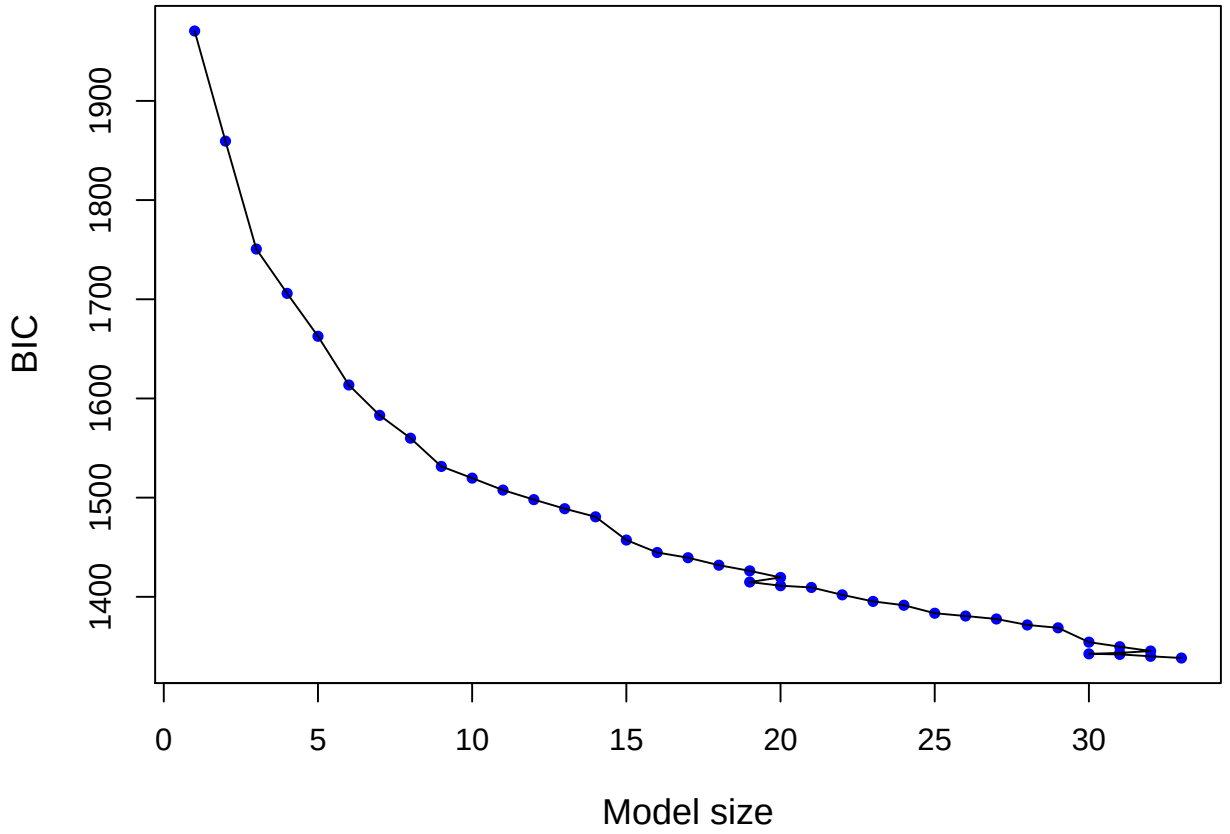
Variable Selection by Stepwise Regression

Diagnostic plot: choice of model

```
> resS <- stepwise(y~X,data=PAC)
```



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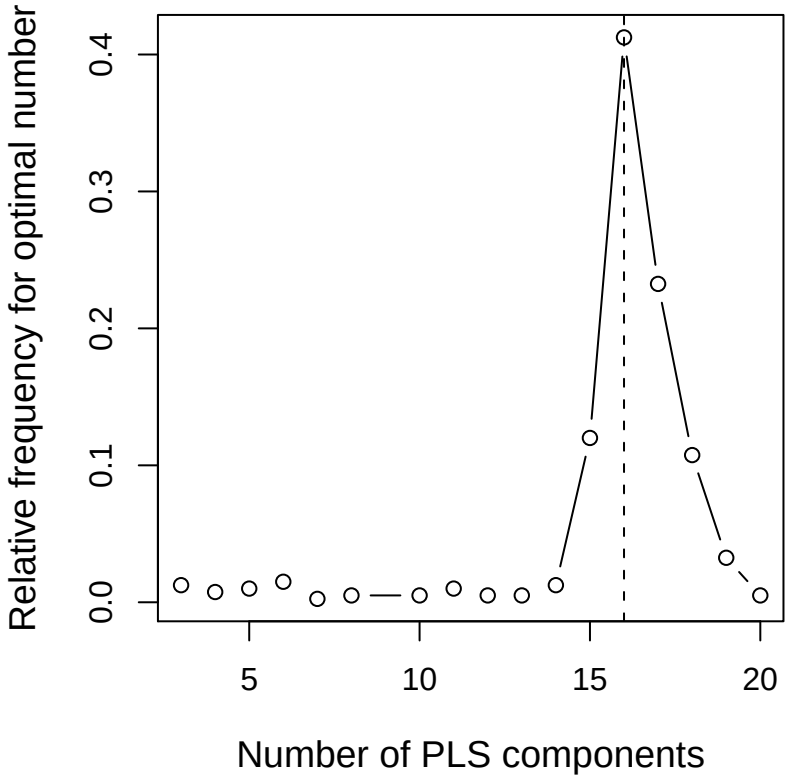
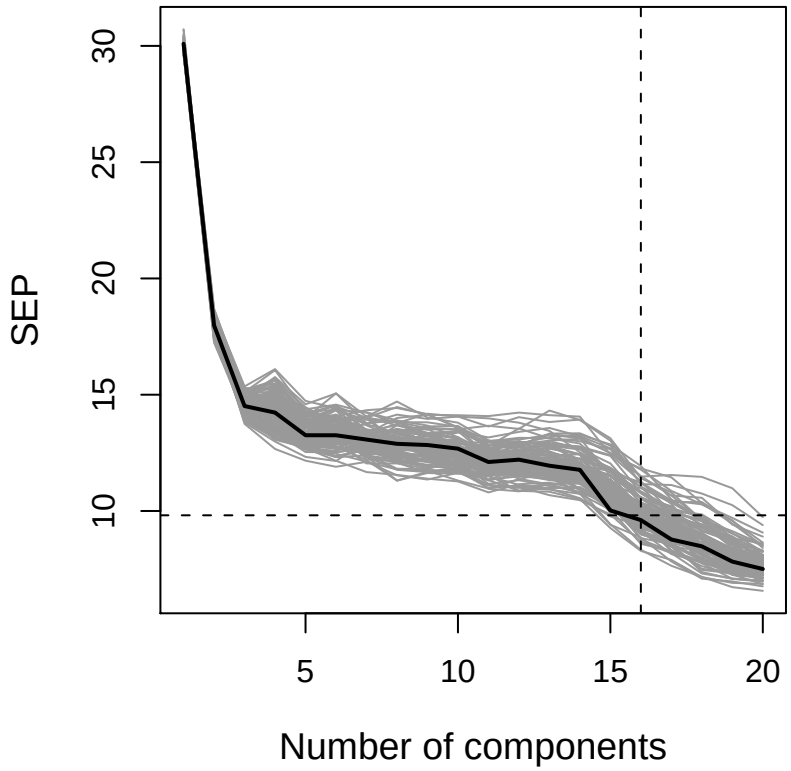
Stepwise Regression + PLS

Diagnostic plot: choice of number of PLS components

```
> resSdcv <- mvr_dcv(y~.,ncomp=20,data=PACred,method="simpls")
```





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Comparison of Results

Method	p^*	k	SEP_{Test}	SEP_{CV}	$SEP^{0.2}$
PCR	467	21	14.2	—	7.9
PLS	467	11	12.0	—	5.7
Robust PLS	467	26	—	8.9	4.0
Ridge regression	467	—	—	28.4	4.0
Lasso regression	145	—	—	7.7	5.0
Stepwise variable selection + PLS	33	16	9.6	—	4.4

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Example data: Origin of glass samples:

- $n = 214$ glass samples
- 6 different glass types (e.g. windows, headlamps, tableware, containers)
- $p = 9$ variables (refractive index, mass-% of Al, Ba, Ca, Fe, K, Mg, Na, Si)

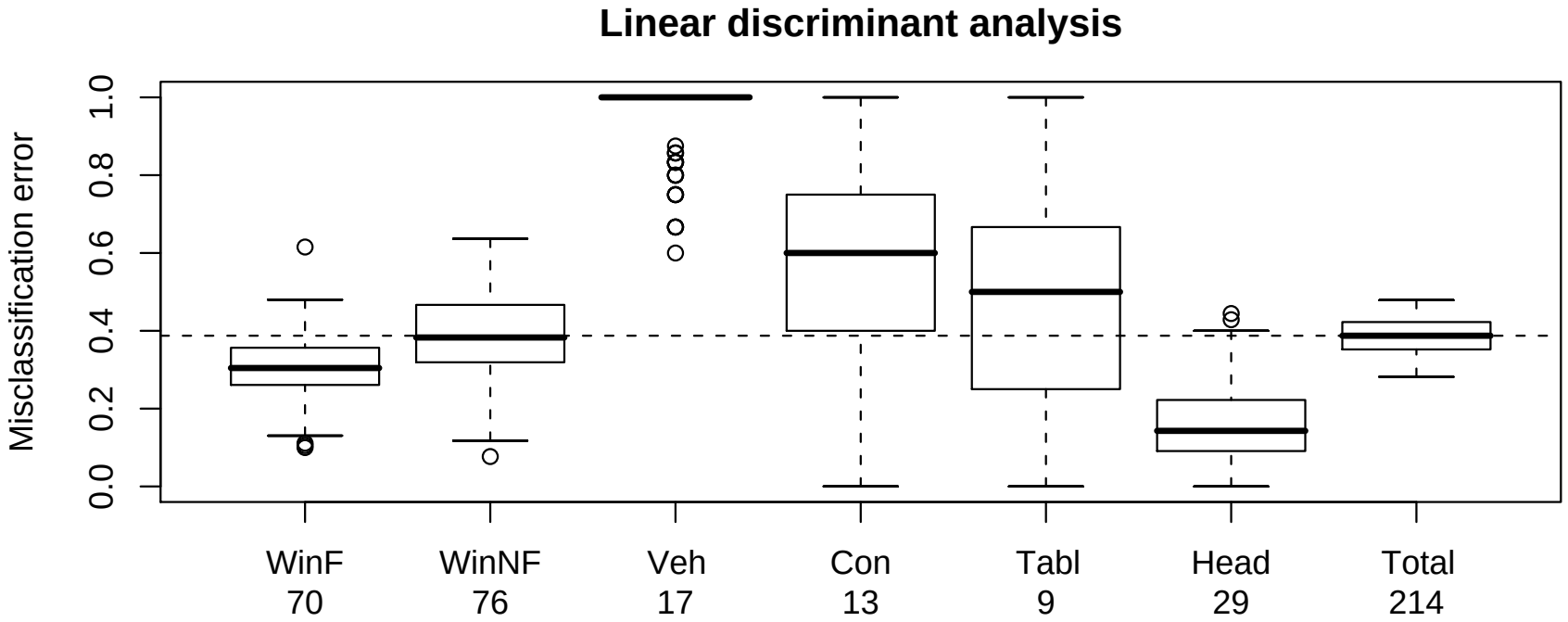
```
> library(MASS)
> data(fgl)
> grp=fgl$type
> X <- scale(fgl[,1:9])
> dim(X)

[1] 214   9
```

LDA (Linear Discriminant Analysis)

LDA: obtain LDA-rule for training data, apply to test data; repeat

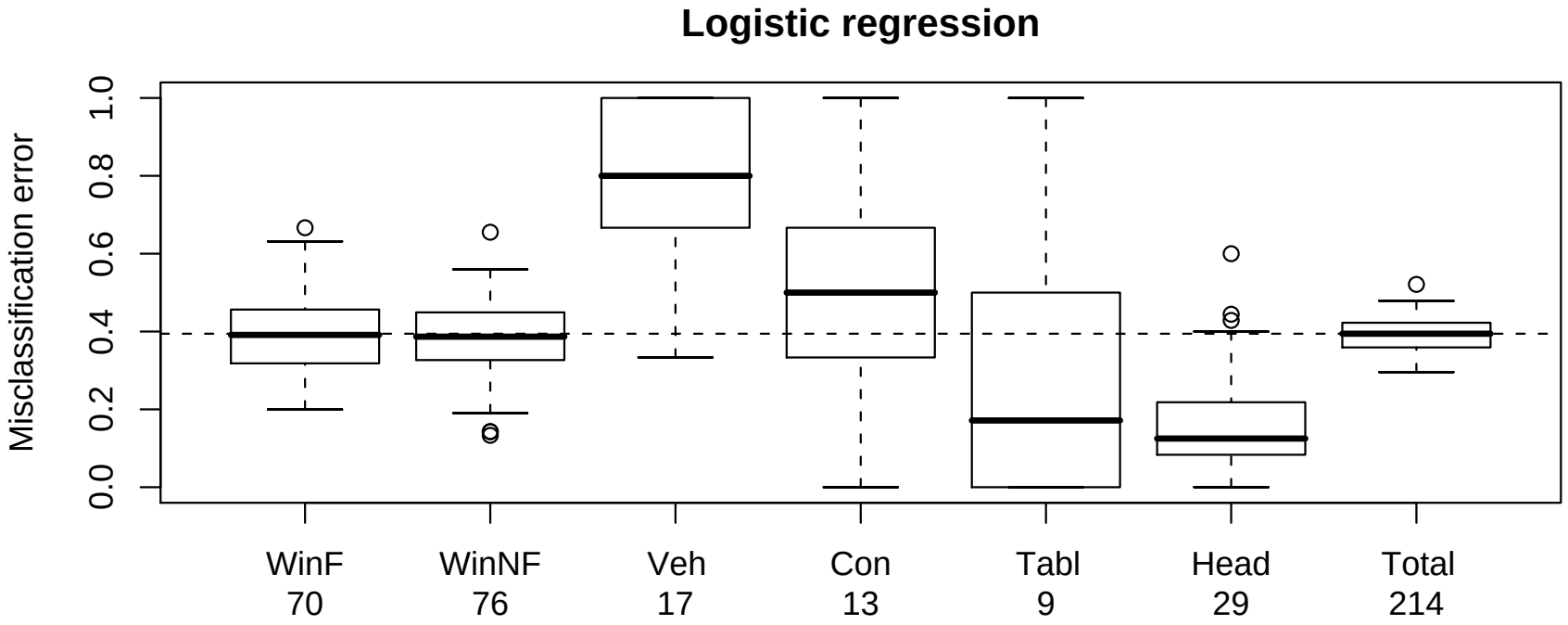
```
> train <- sample(1:n,ntrain)
> reslda <- lda(X[train,],grp[train])
> pred <- predict(reslda,newdata=X[-train,])$class
> tab <- table(grp[-train],pred)
```



LR (Logistic Regression)

LR: obtain LR-rule for training data, apply to test data; repeat

```
> train <- sample(1:n,ntrain)
> reslr <- vglm(grp ~ .,data=dat[train,],family=multinomial)
> predmix <- predict(reslr,dat[-train,],type="response")
> predgrp <- apply(predmix,1,which.max)
> tab <- table(grp[-train],predgrp)
```



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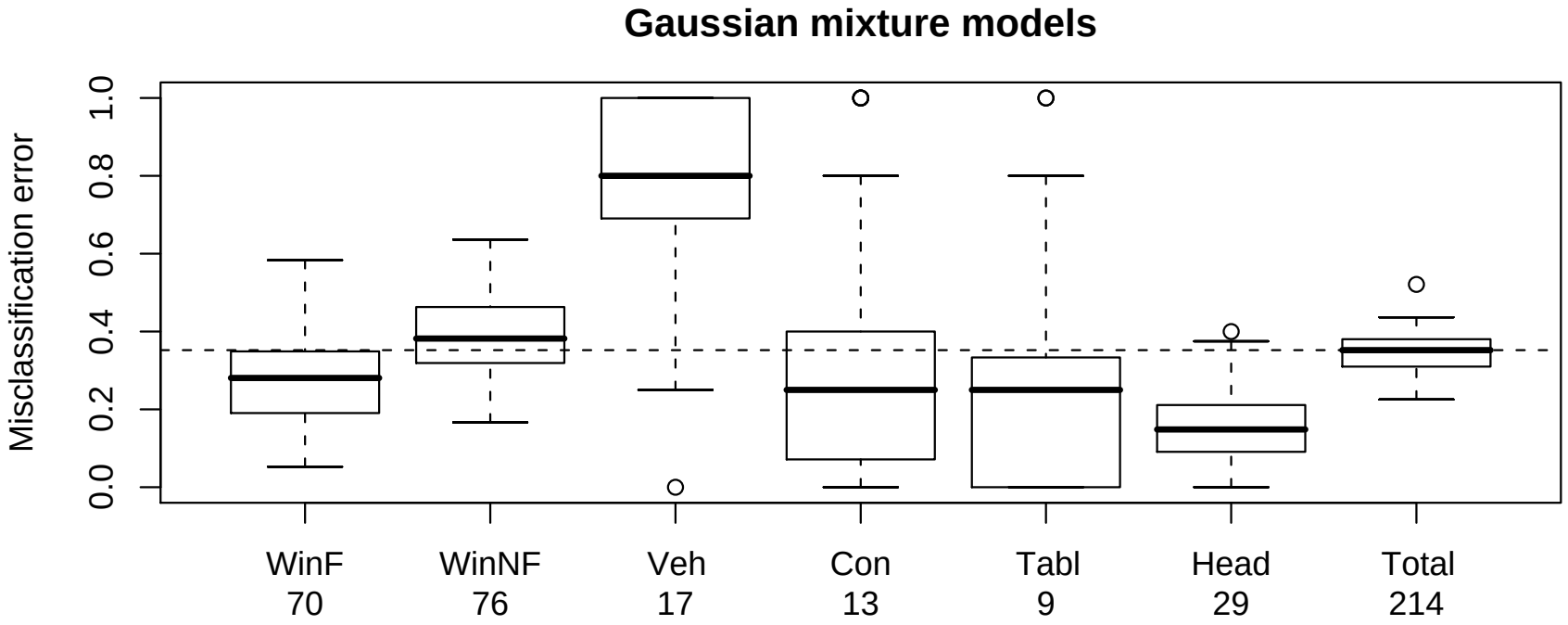
Mix: Gaussian Mixture Models

Mix: obtain models for training data, apply to test data; repeat

```
> train <- sample(1:n,ntrain)
> resgmm <- mda(grp ~ .,data=dat[train,])
> predgmm <- predict(resgmm,dat[-train,],type="post")
> predgrp <- apply(predgmm,1,which.max)
> tab <- table(grp[-train],predgrp)
```



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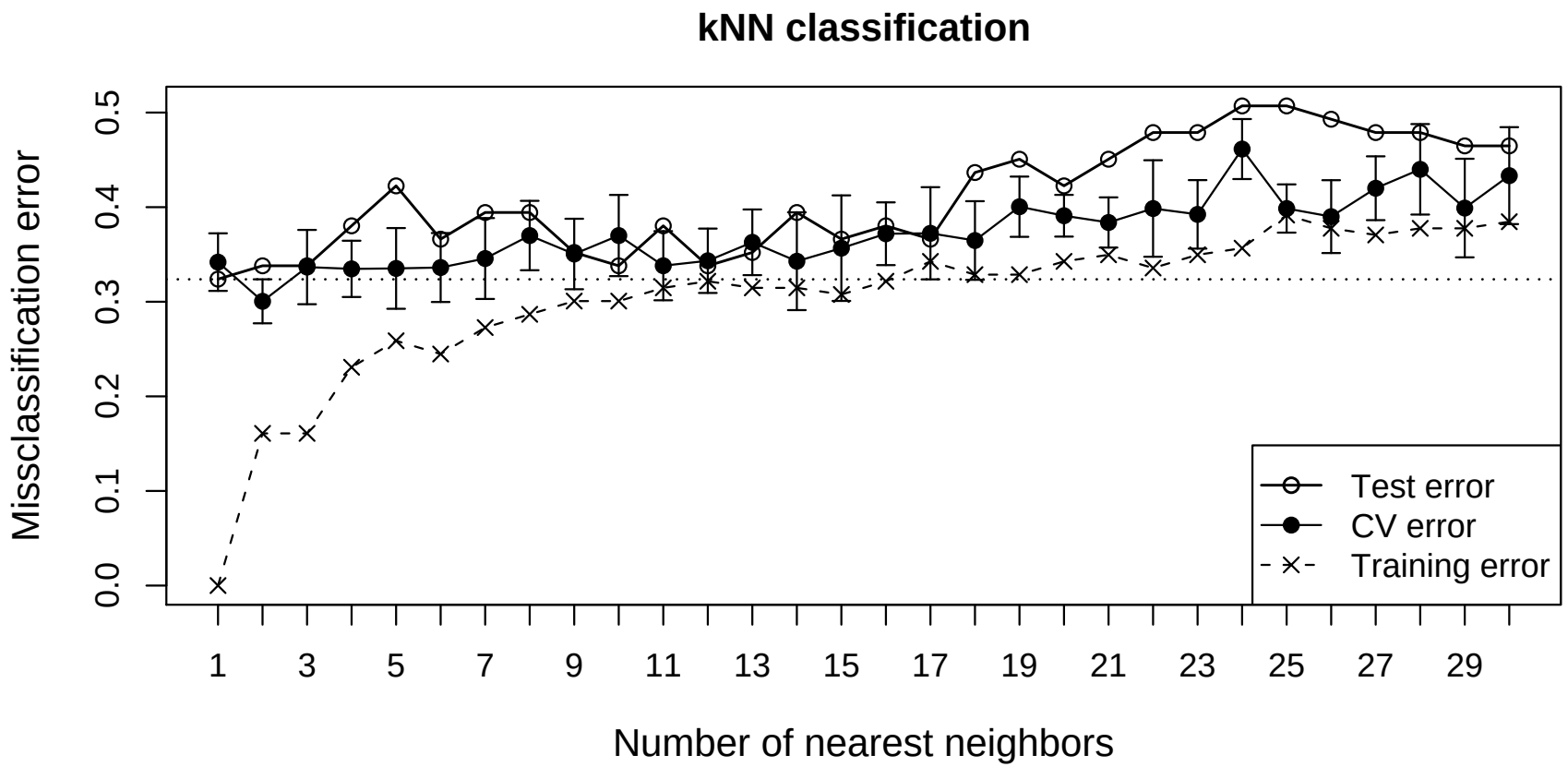
kNN: k-nearest-neighbor classification

kNN: select tuning parameter “k” (number of neighbors)

```
> train <- sample(1:n,ntrain)
> resknn <- knnEval(X,grp,train,knnvec=seq(1,30,by=1))
```



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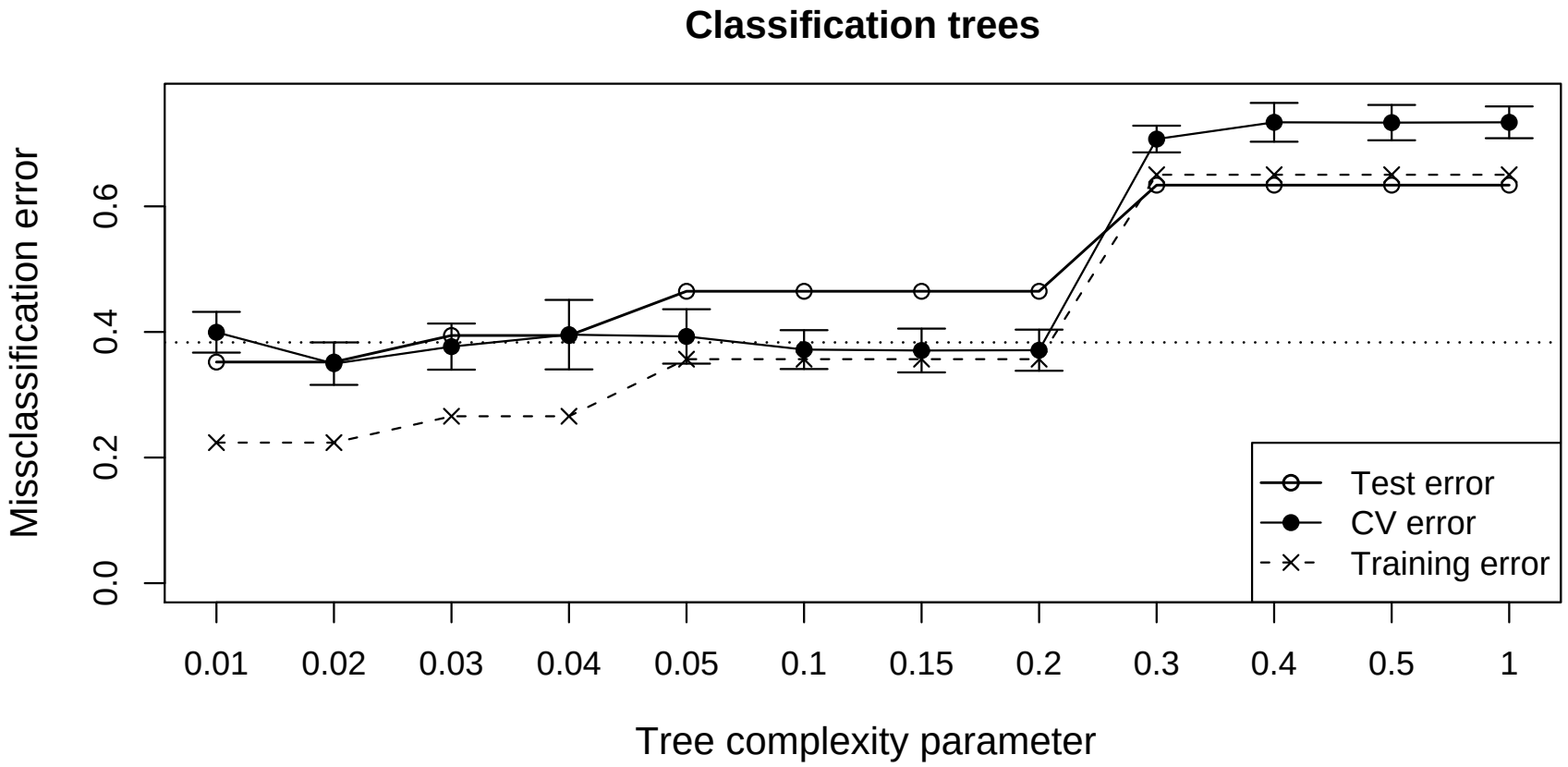
Tree: classification trees

Tree: select tuning parameter “cp” (tree complexity)

```
> train <- sample(1:n,ntrain)
> cptry <- c(0.01,0.02,0.03,0.04,0.05,0.1,0.15,0.2,0.3,0.4,0.5,1)
> restree <- treeEval(X,grp,train,cp=cptry)
```



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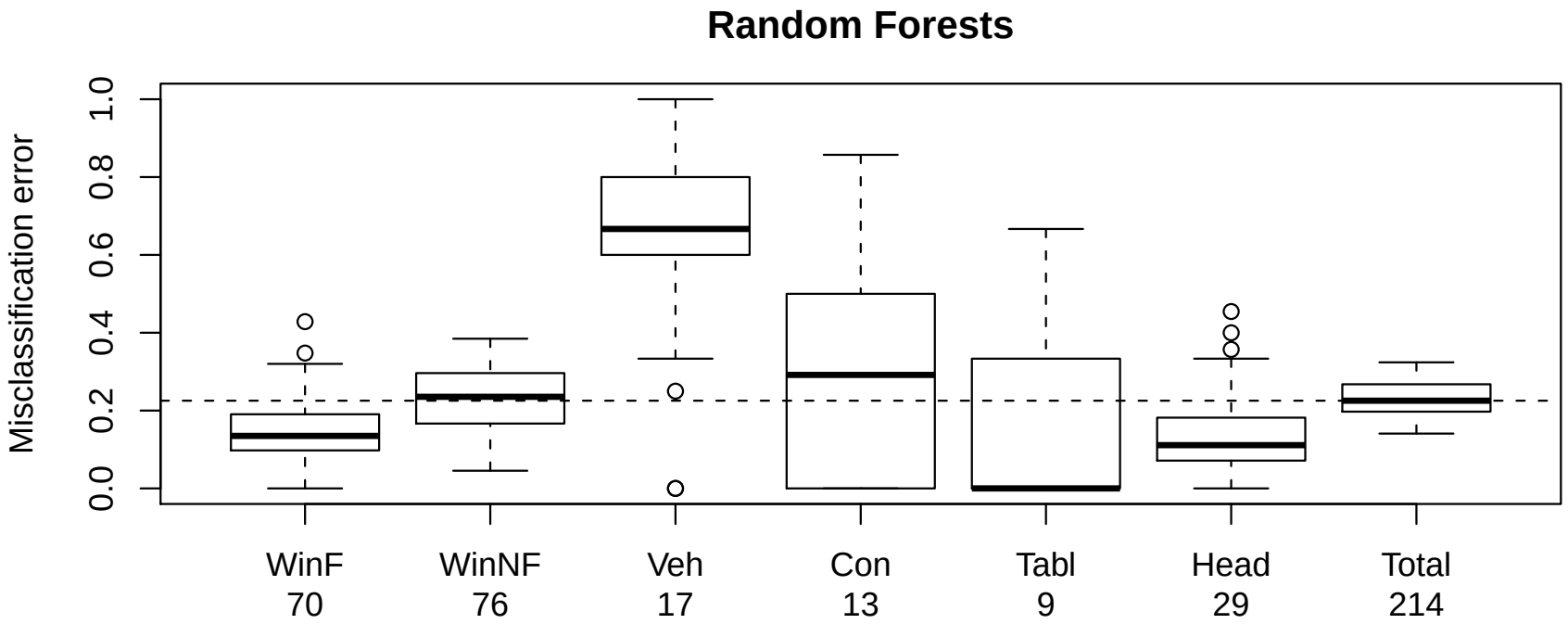
RF: Random Forests

RF: obtain rule for training data, apply to test data; repeat

```
> train <- sample(1:n,ntrain)
> resRF <- randomForest(grp~.,data=dat,subset=train)
> predRF <- predict(resRF, dat[-train,])
> table(grp[-train],predRF)
```



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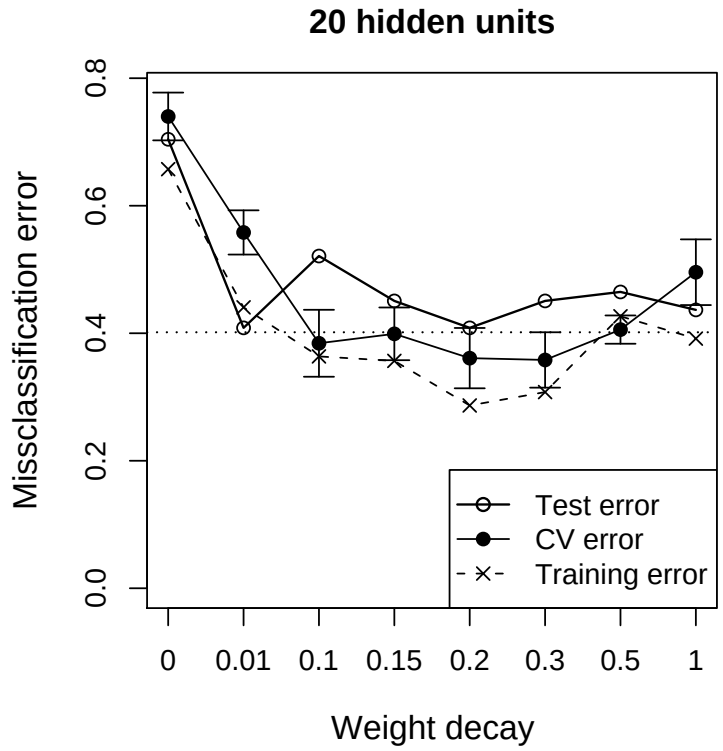
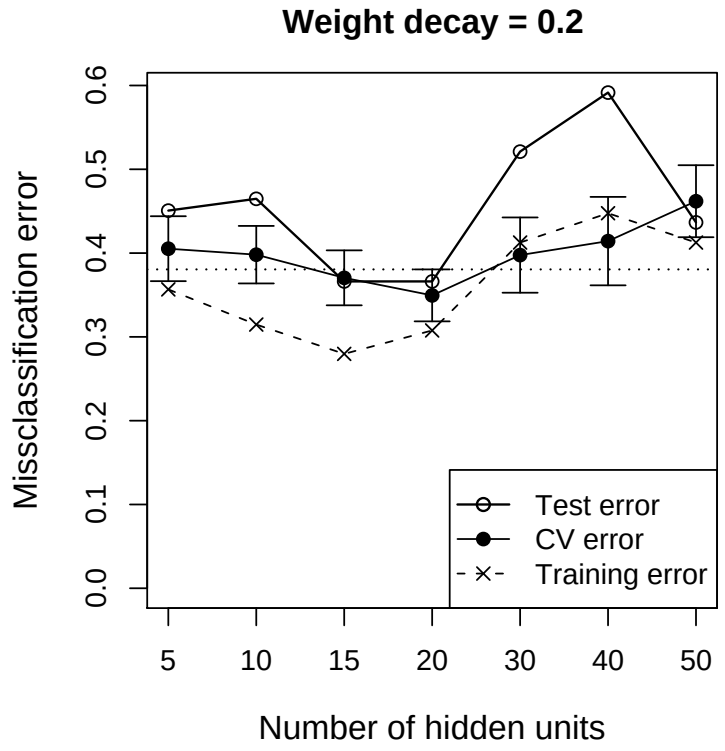
ANN: Artifician Neural Networks

ANN: select tuning parameters “weight decay” and “number of hidden units”

```
> train <- sample(1:n,ntrain)
> wd <- c(0,0.01,0.1,0.15,0.2,0.3,0.5,1)
> sz <- c(5,10,15,20,30,40,50)
> resnnet=nnetEval(X,grp,train,decay=wd,size=20)
> resnnet=nnetEval(X,grp,train,decay=0.2,size=sz)
```





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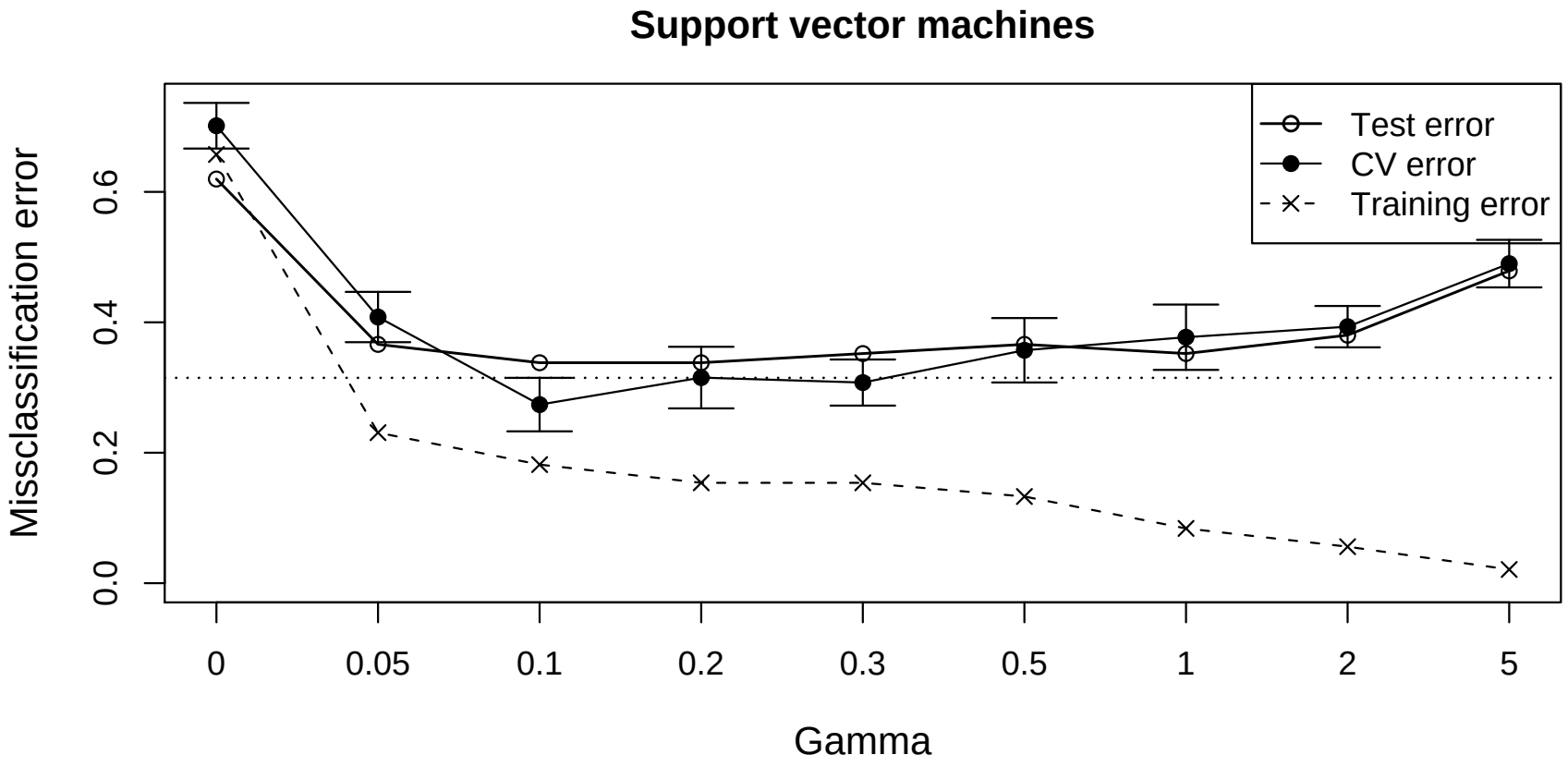
SVM: Support Vector Machines

SVM: select tuning parameter "γ" (size constraint of slack variables)

```
> train <- sample(1:n,ntrain)
> gv <- c(0,0.05,0.1,0.2,0.3,0.5,1,2,5)
> ressvm <- svmEval(X,grp,train,gamvec=gv)
```



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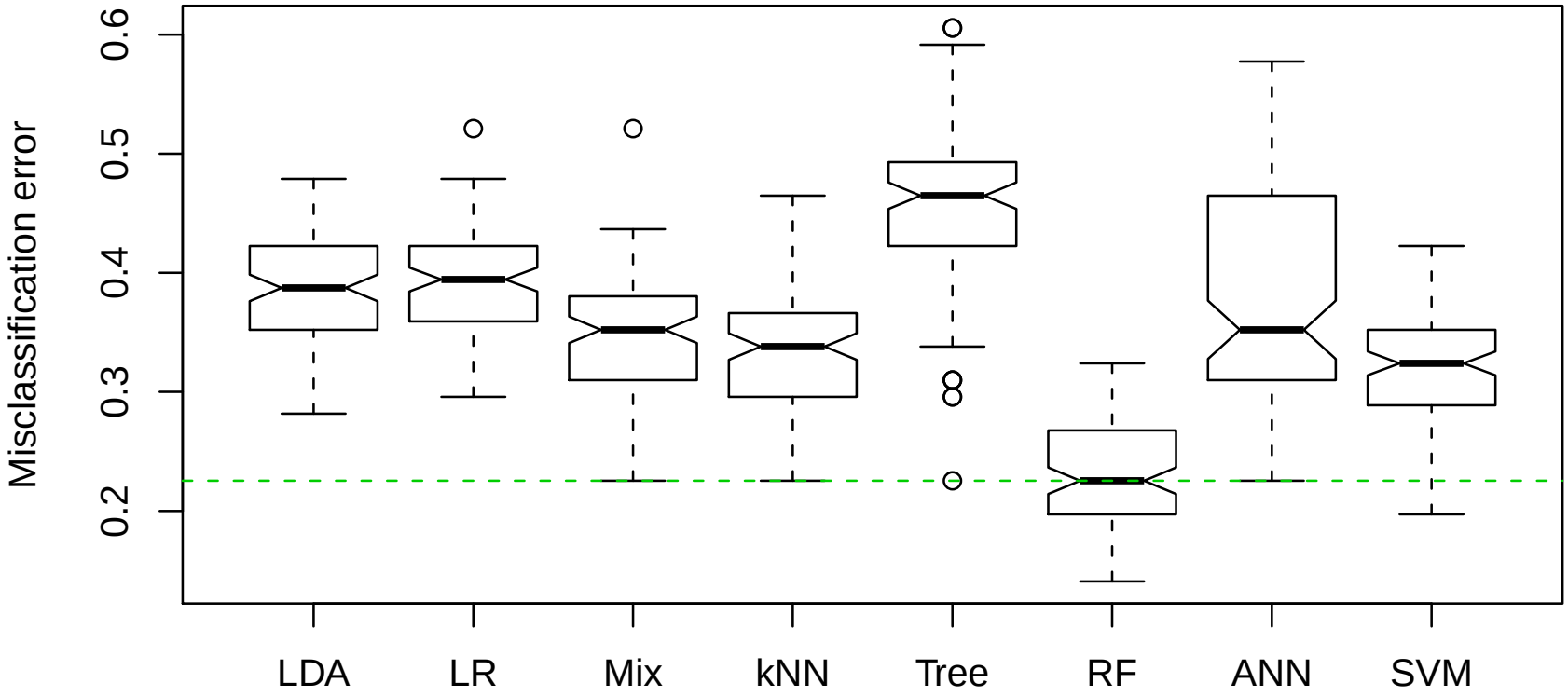
Overall Comparison



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Conclusions

- The book is not only suitable for chemometricians, but for all who want to learn about **multivariate statistical methods** from a theoretical and practical perspective.

- Data sets and methods treated in the book are included in the R package **chemometrics**. The different evaluation procedures (*repeated cross validation*) are implemented in a unified manner.

- We already received a lot of positive feedback to both, the book and the R package.

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