The "chemometrics" Package in R – Application in Multivariate Calibration and Classification

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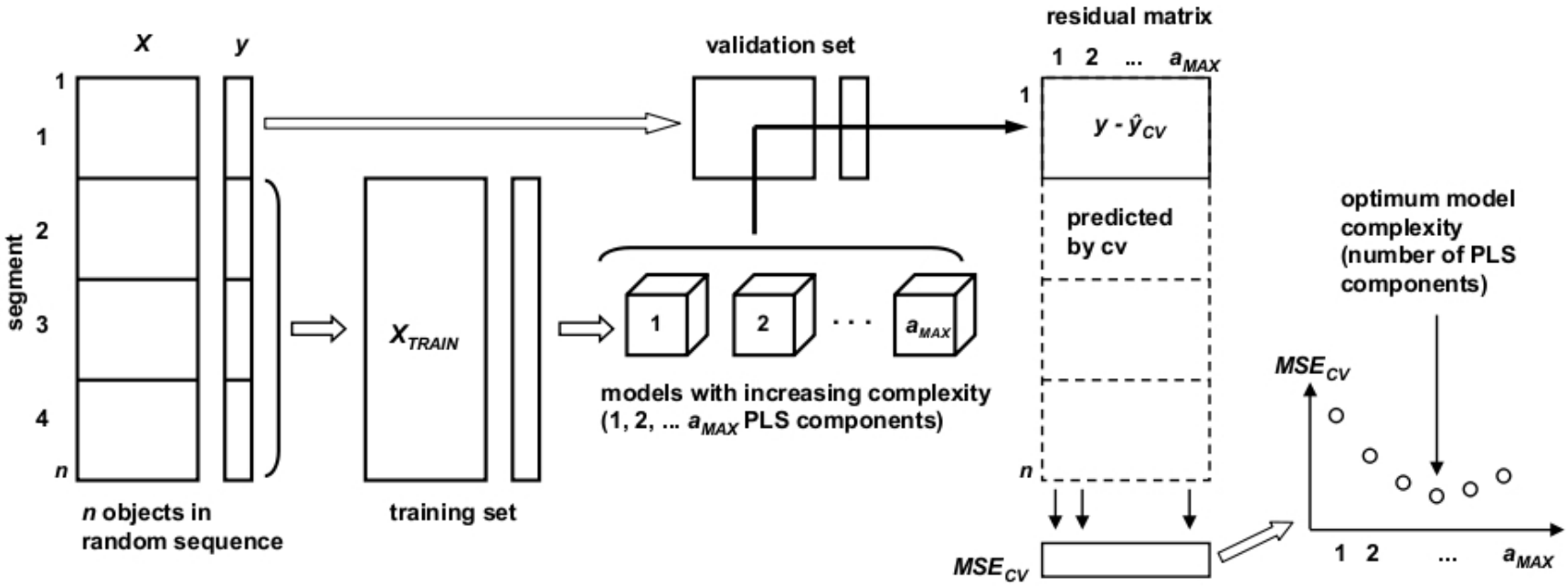
What is available in R?

. . . nearly "everything" with respect to multivariate calibration and classification. For calibration, the package "pls" is very valuable.

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

Cross Validation



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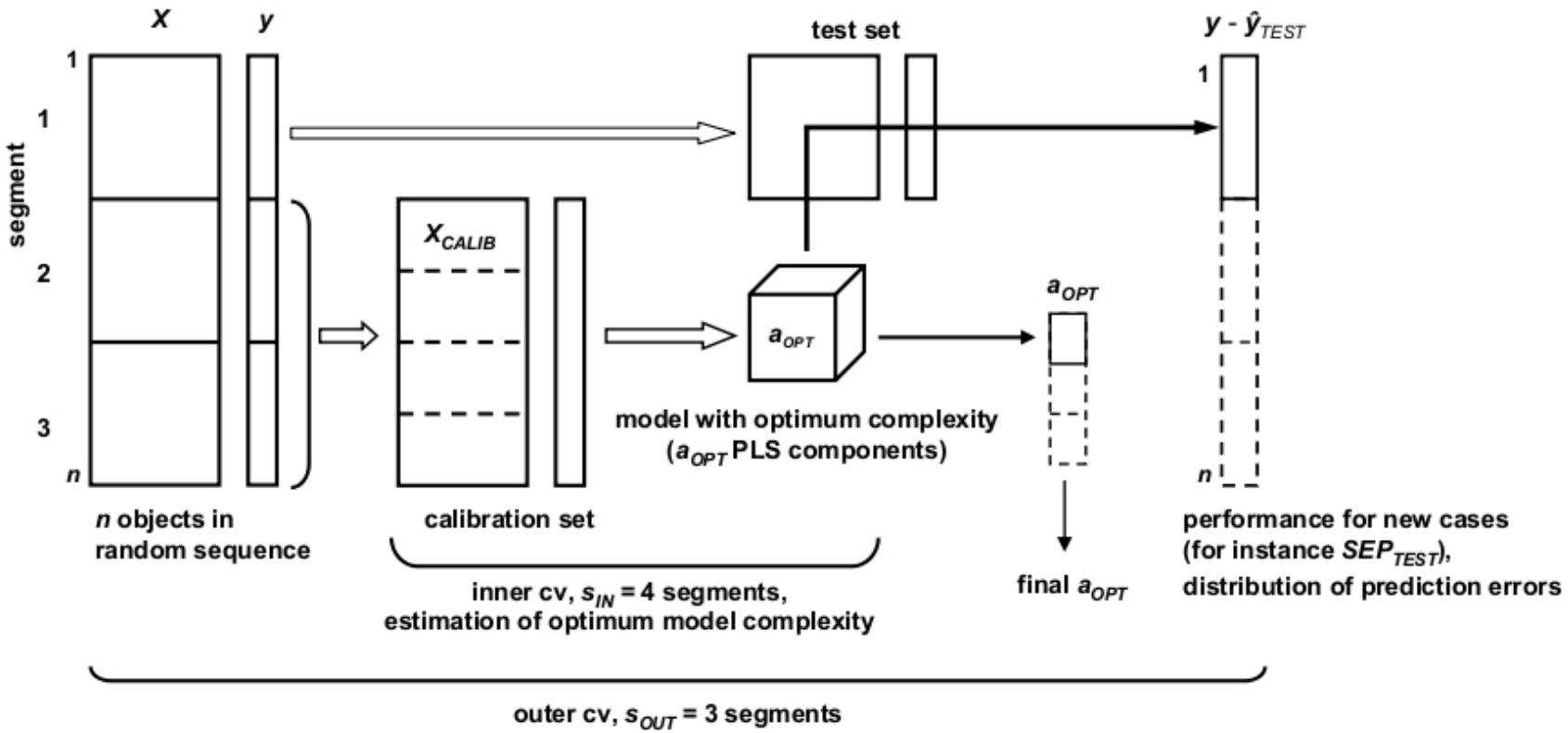
Repeated Double Cross Validation



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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: $m = 467$ 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"
```

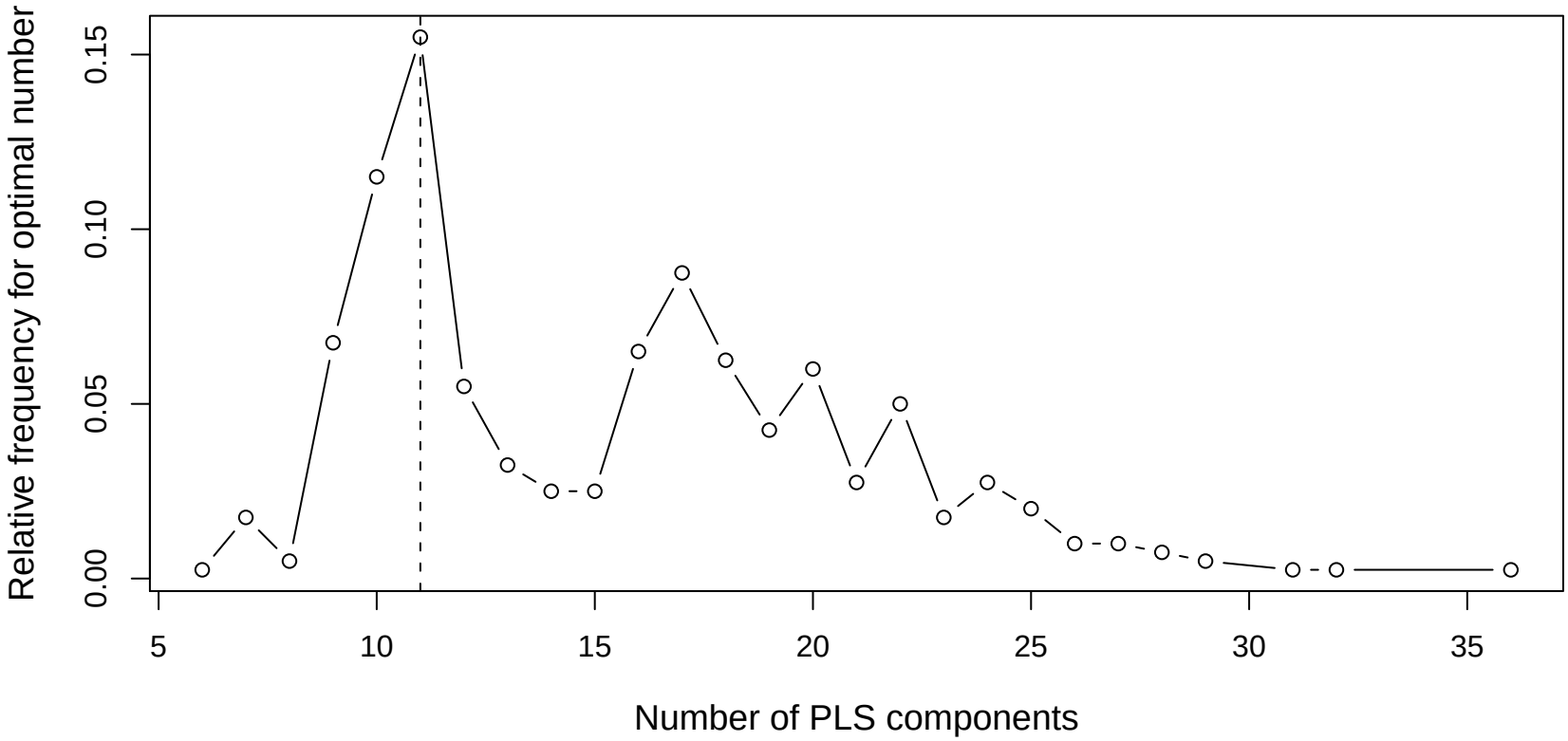
Output:

```
 $ 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]
```

PLS (and PCR)

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

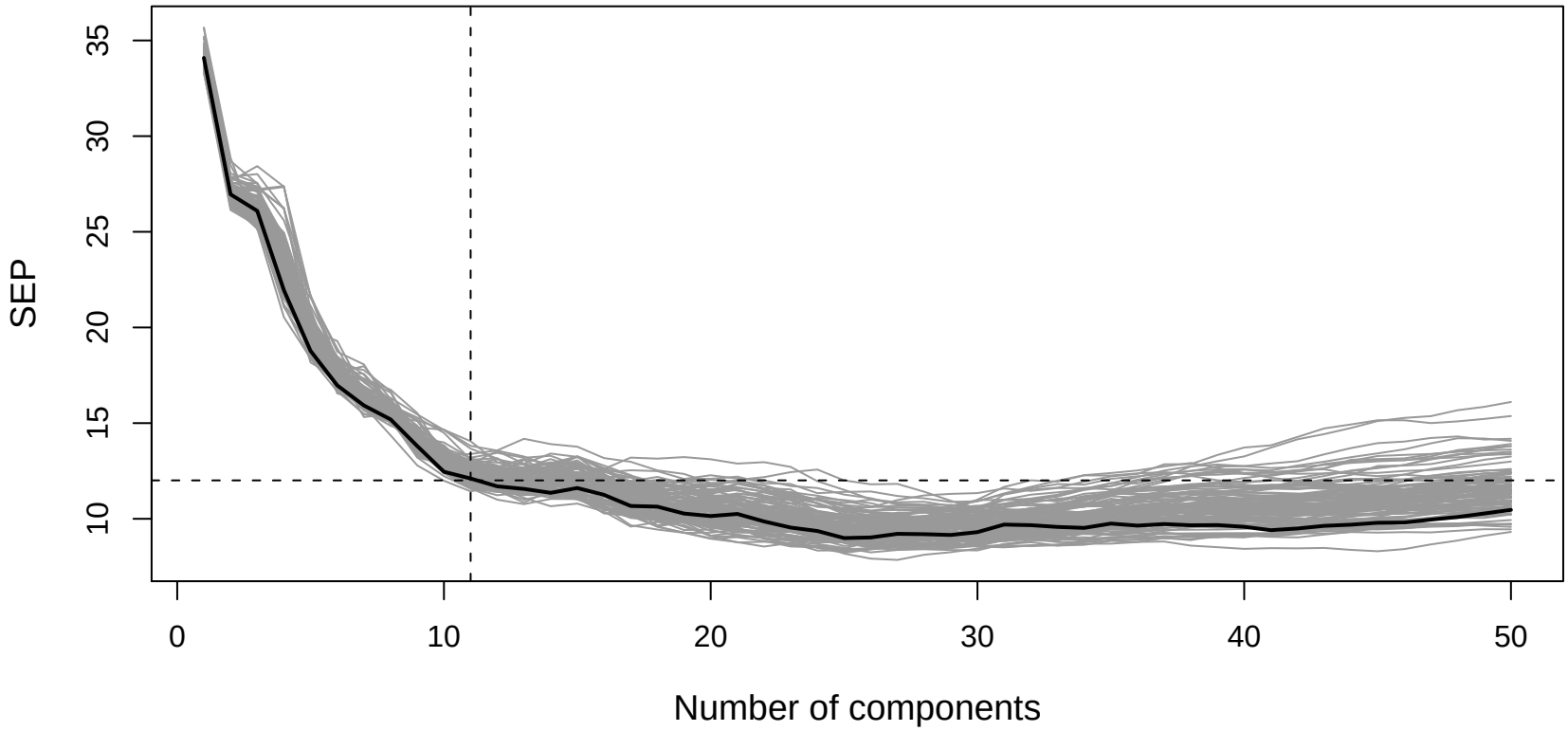
```
> plotcompmvr(pls_dcv)
```



PLS (and PCR)

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

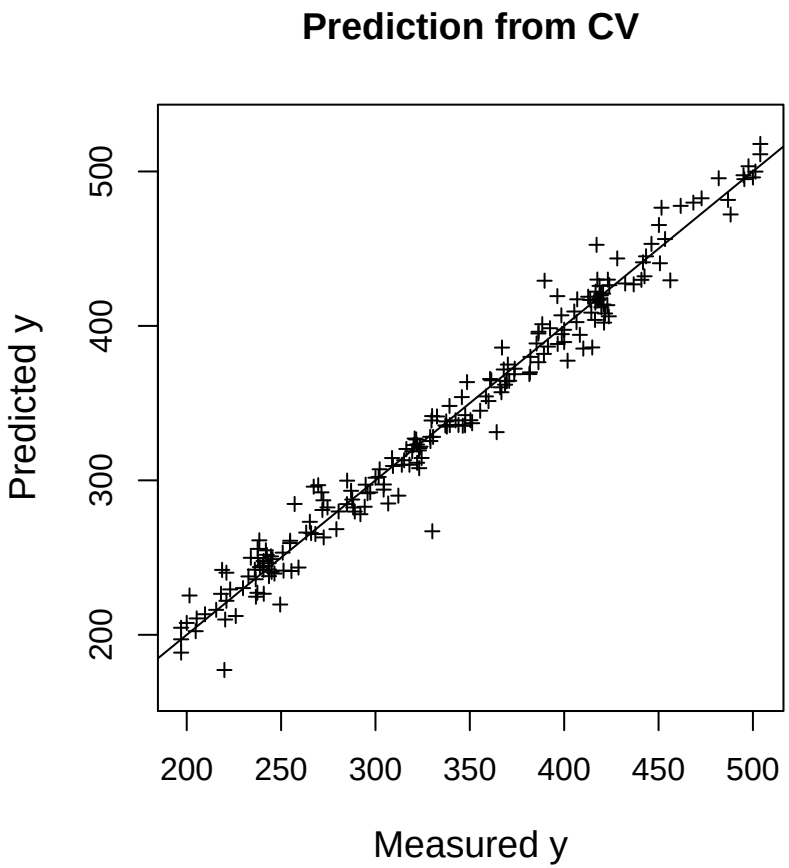
```
> plotSEPmvr(pls_dcv,optcomp=11,y=PAC$y,X=PAC$X,method="simpls")
```

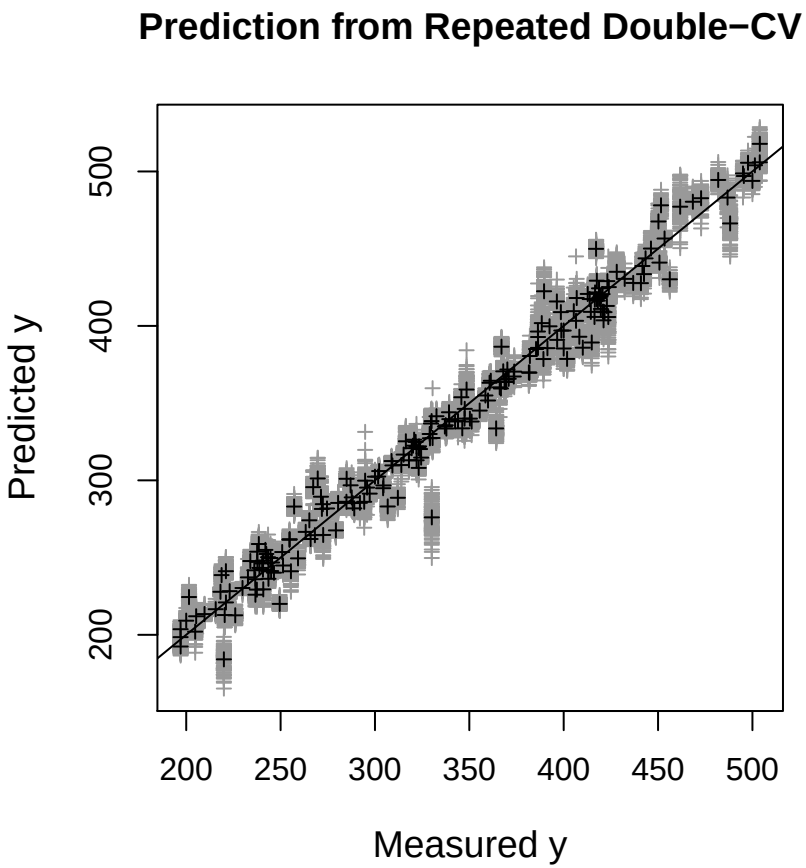


PLS (and PCR)

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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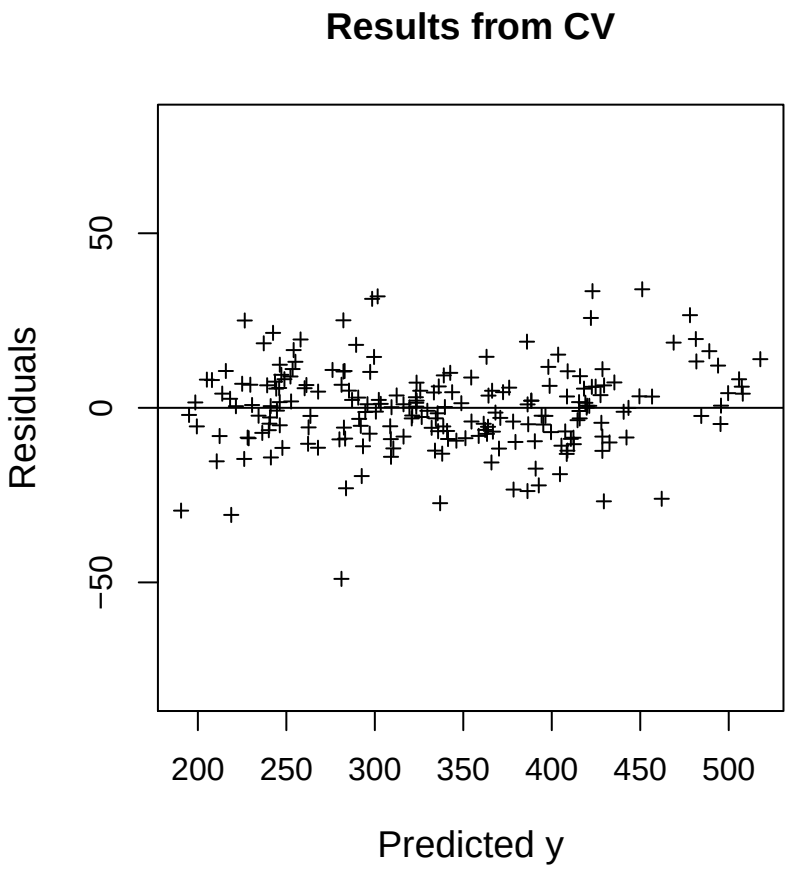
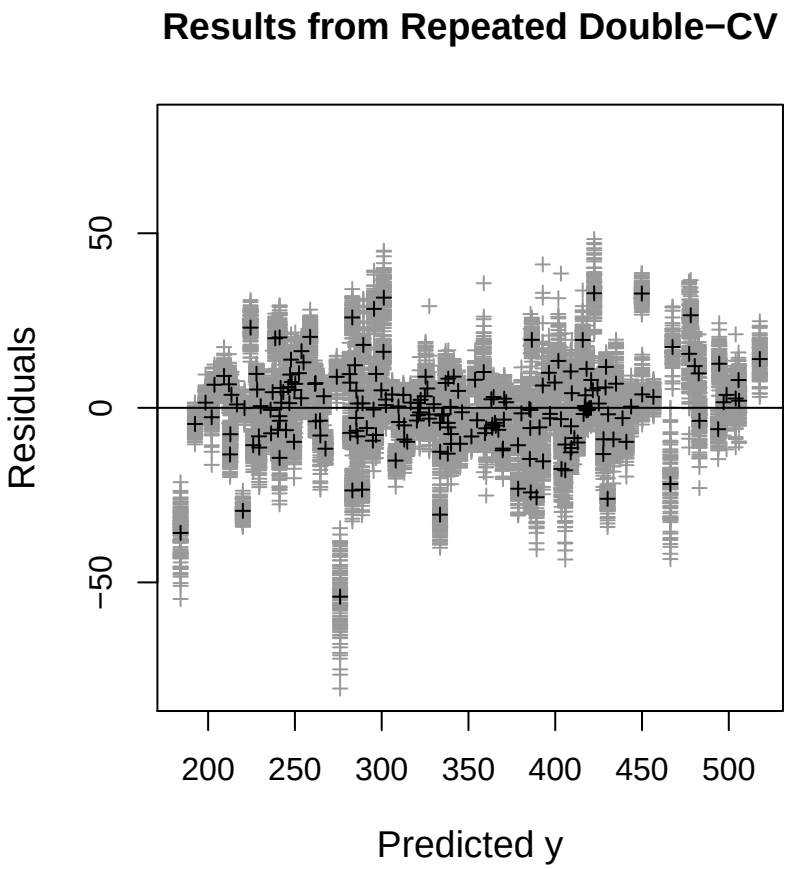
PLS (and PCR)

Diagnostic plots: residuals from 100 models with 11 components

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

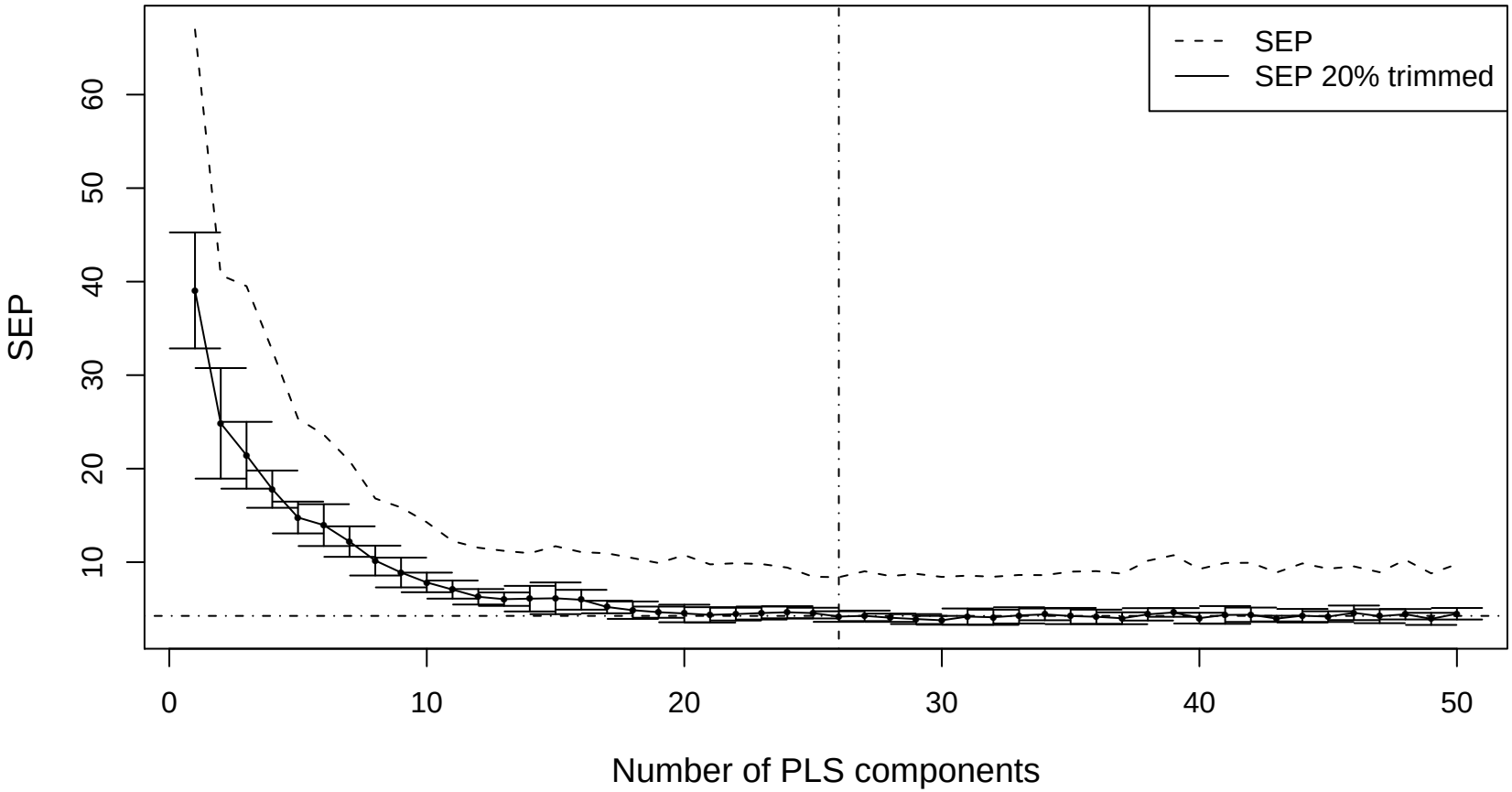




Robust PLS

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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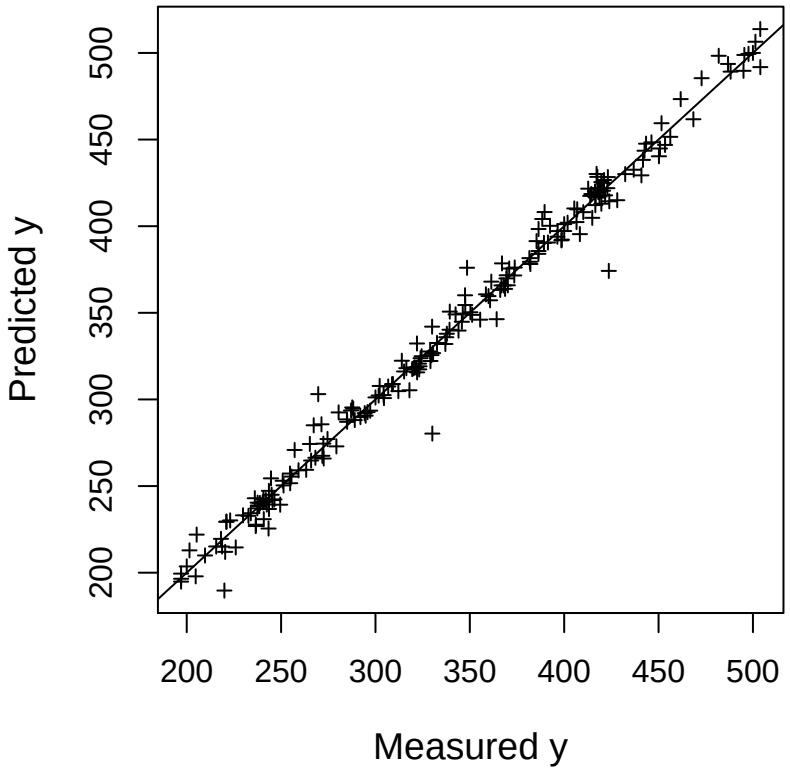
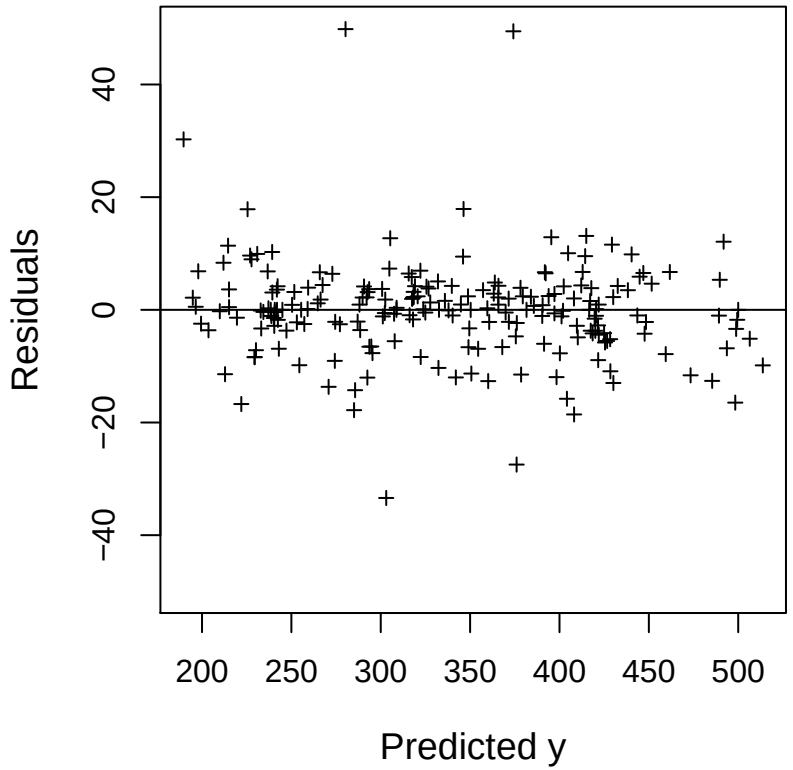
Robust PLS

Diagnostic plots: predicted values and residuals using 26 components

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





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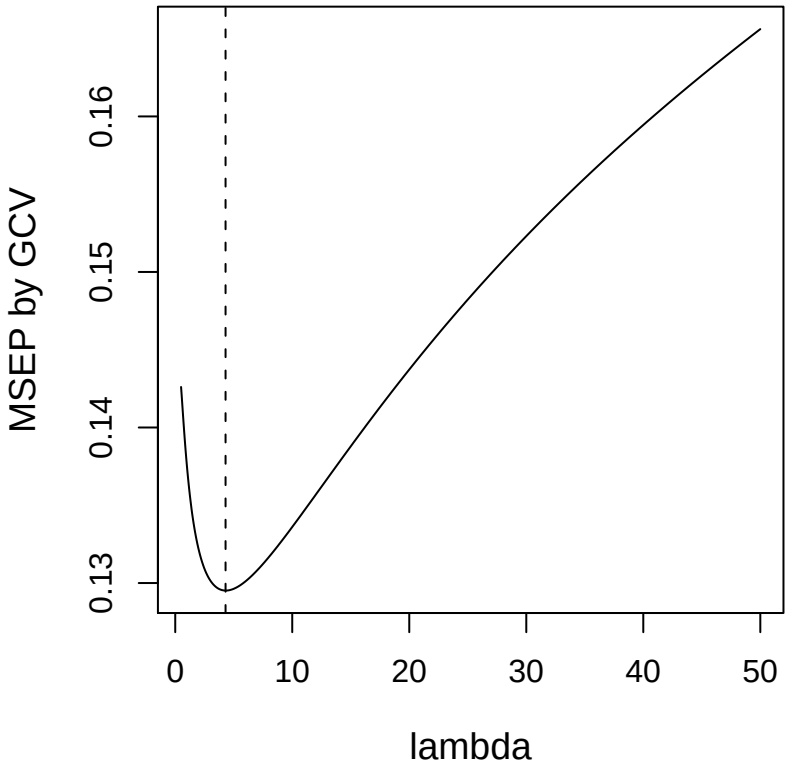
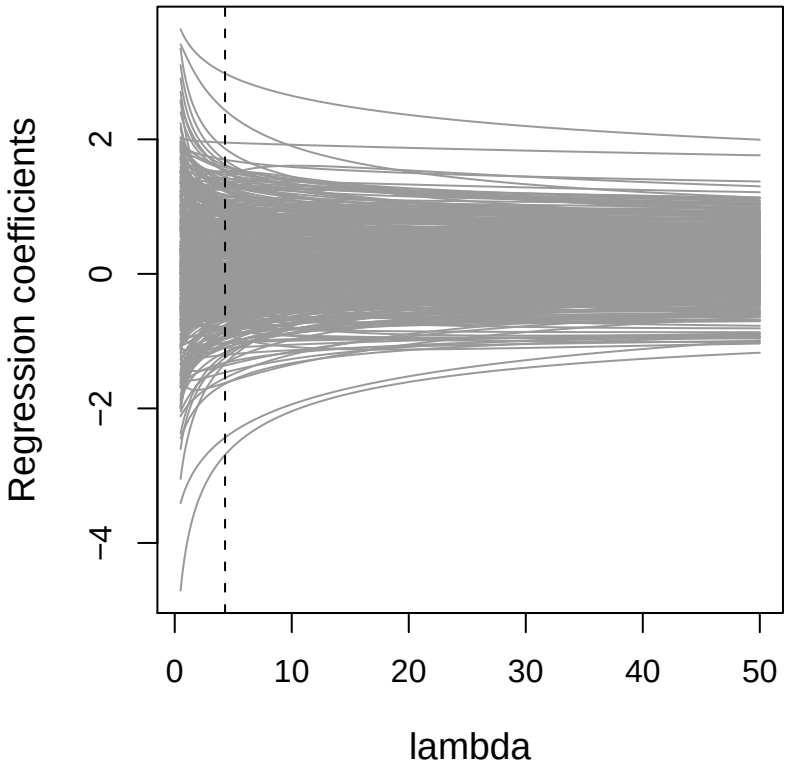
Ridge Regression

Diagnostic plot: choice of ridge parameter

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





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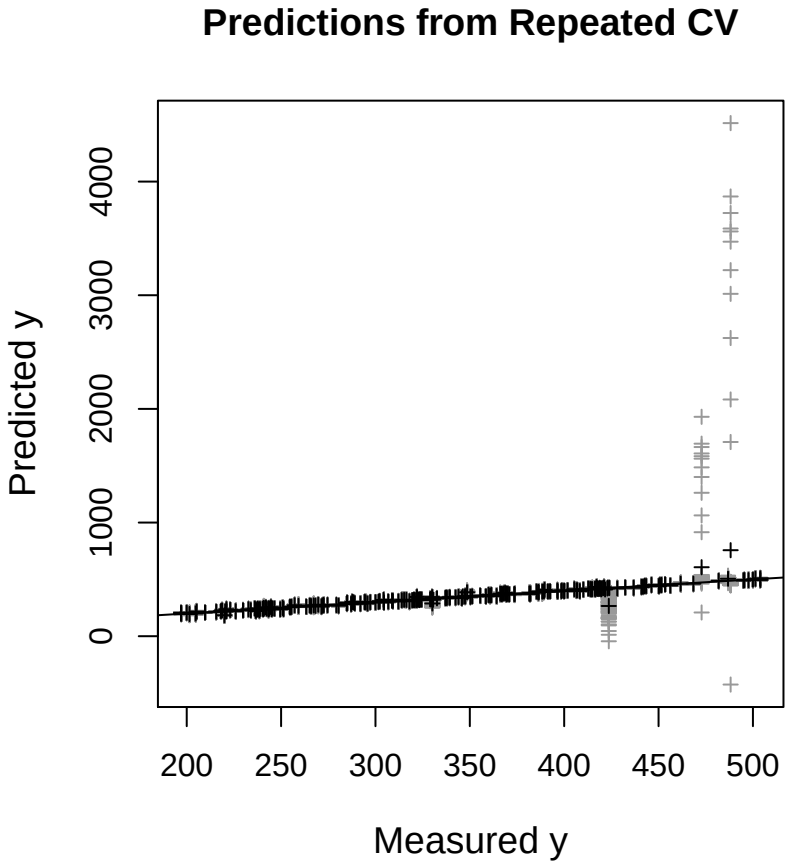
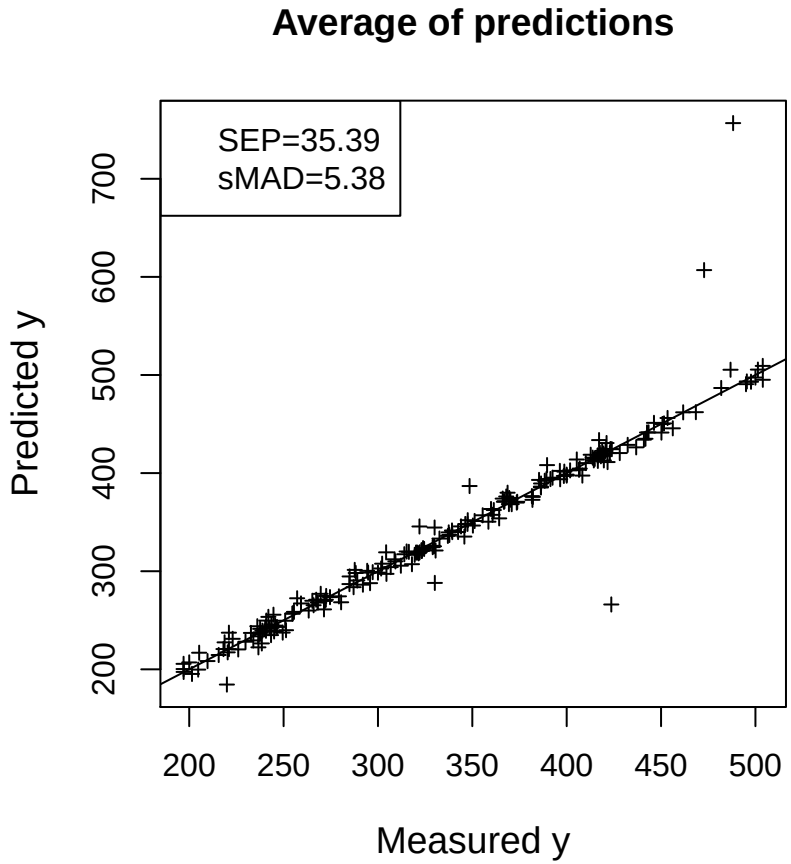
Ridge Regression

Diagnostic plots: from repeated cross validation

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

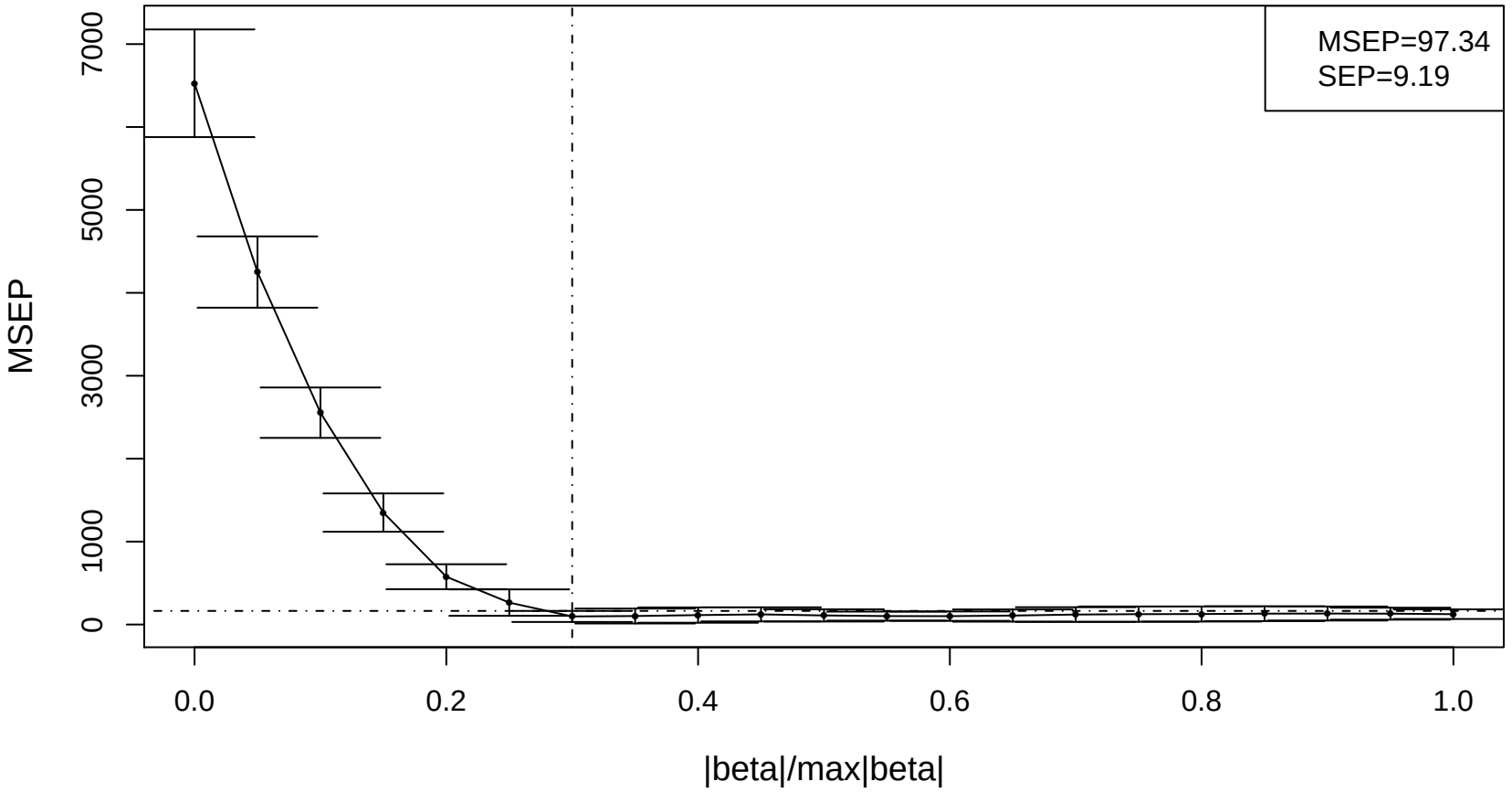




Lasso Regression

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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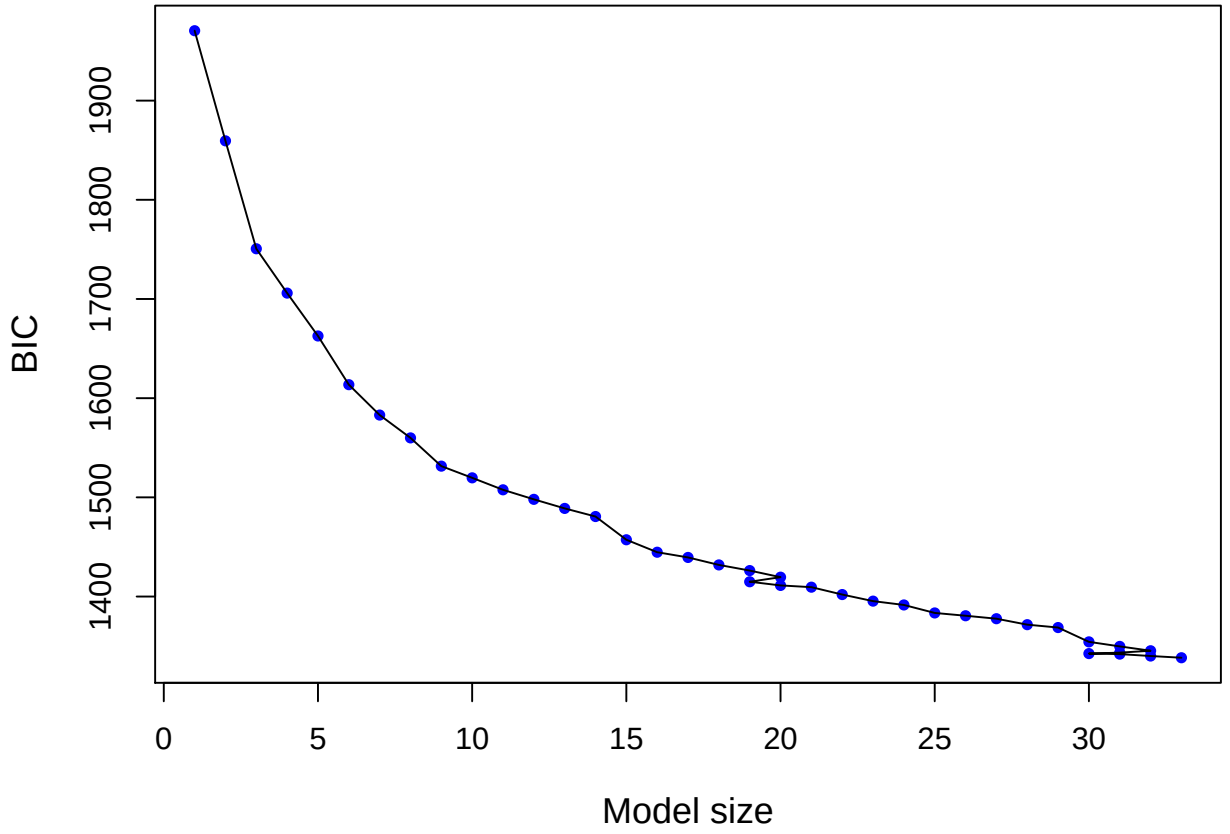
Variable Selection by Stepwise Regression

Diagnostic plot: choice of model

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



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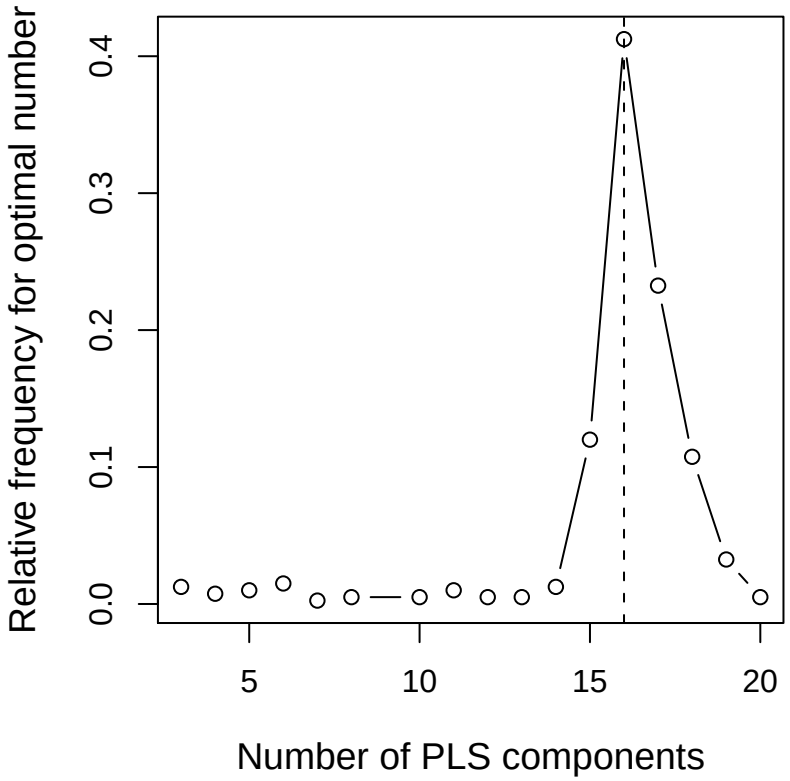
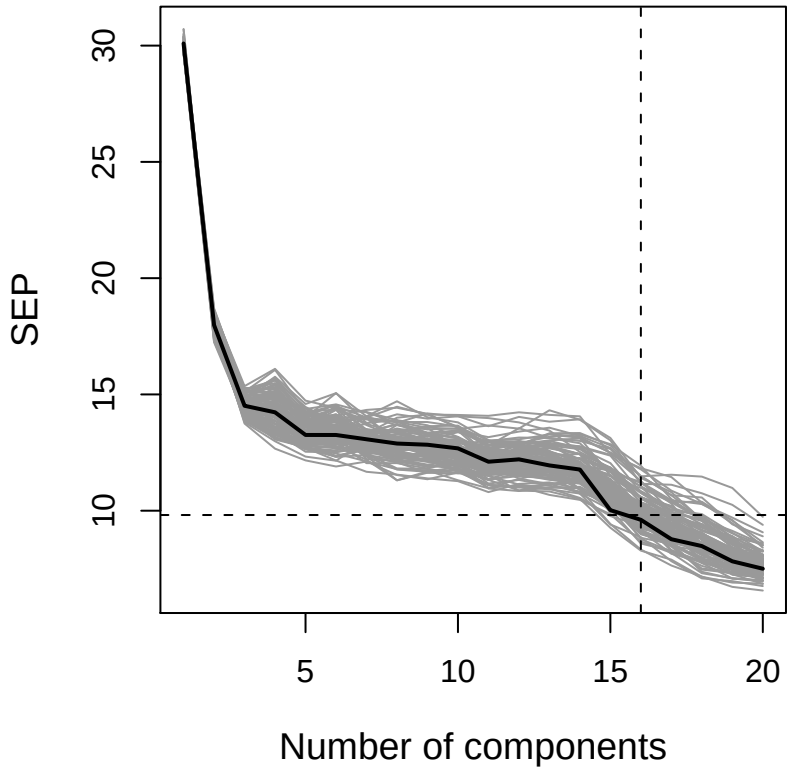
Stepwise Regression + PLS

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	**m***	**a**	**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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Classification Methods

- **Linear classification methods:** linear discriminant analysis (LDA), logistic regression (LR)
- **Kernel and prototype methods:** Gaussian mixture models, k-NN classification
- **Classification trees and random forests**
- **Artficial neural networks**
- **Support vector machines**
- ...

Multivariate Classification

Example data: Origin of glass samples:

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

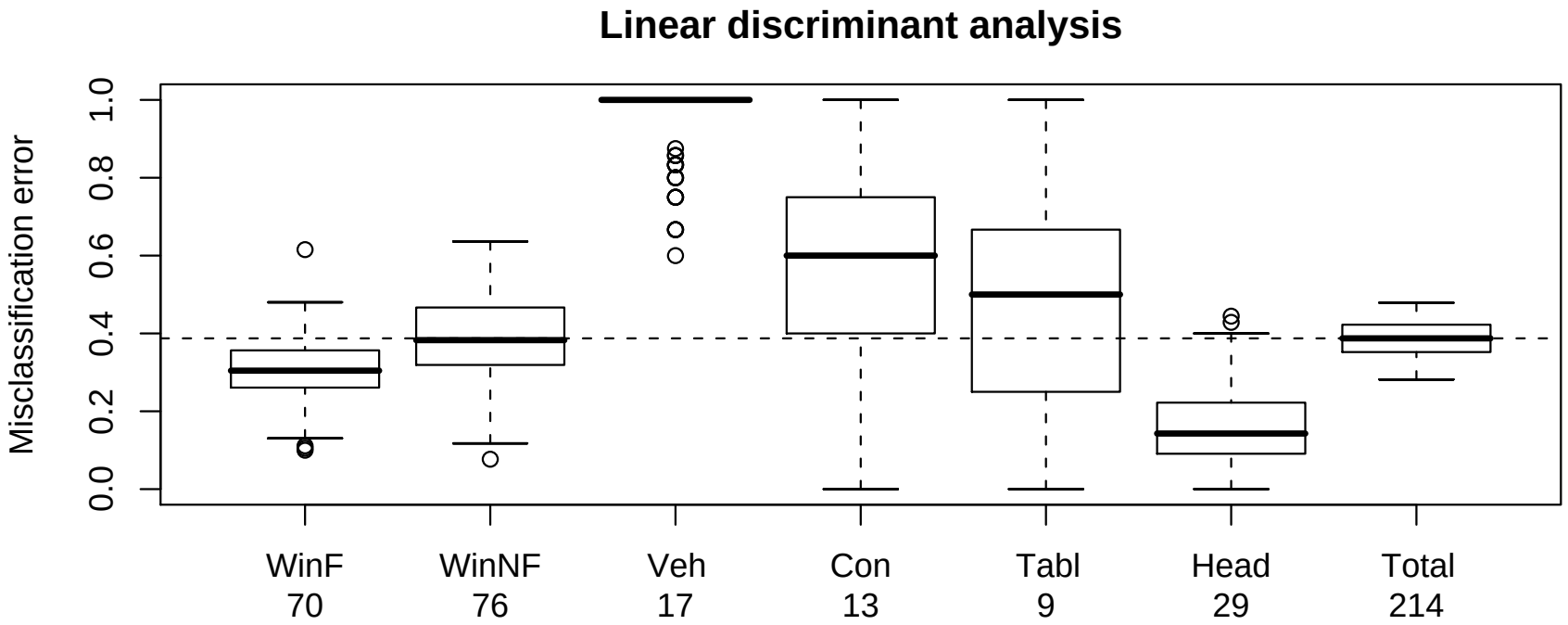
```
> library(MASS)
> data(fgl)
> grp=fgl$type
> X <- scale(fgl[,1:9])
> dim(X)

[1] 214   9
```

LDA (Linear Discriminant Analysis)

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

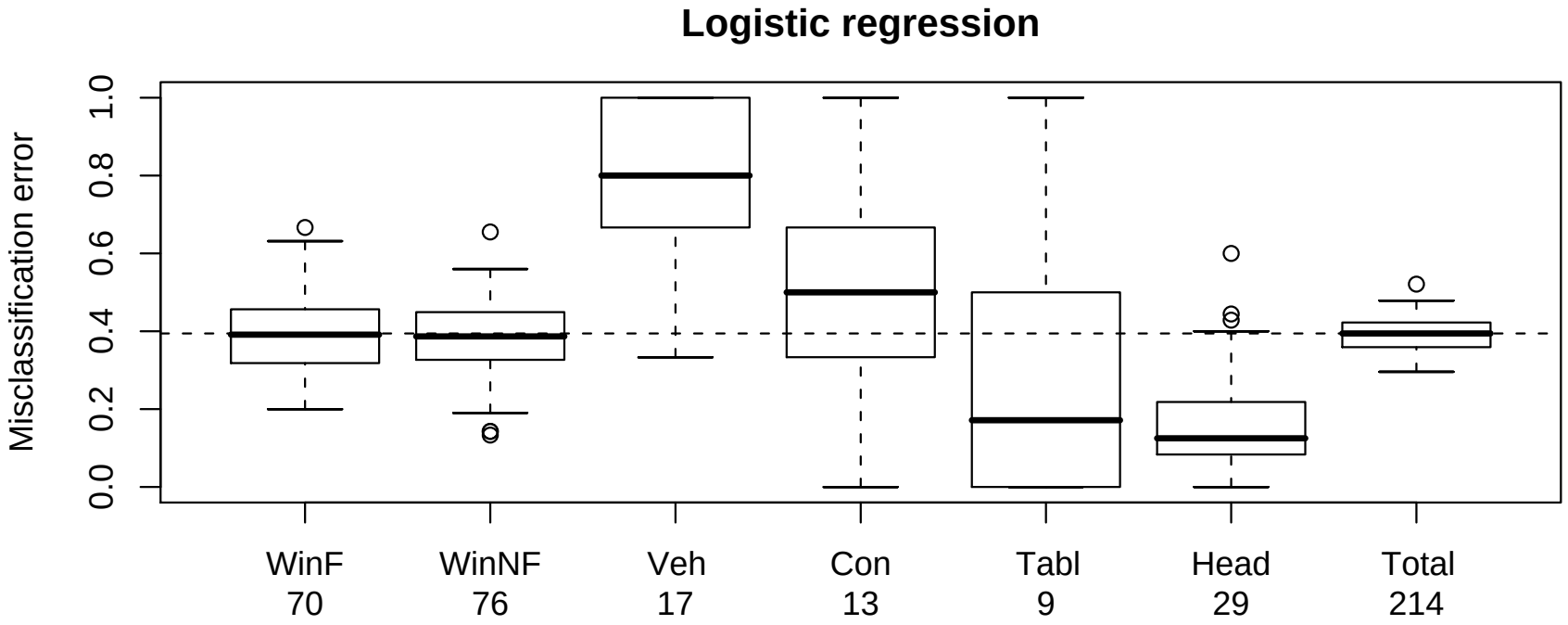
```
> train <- sample(1:n,ntrain)
> reslda <- lda(X[train,],grp[train])
> pred <- predict(reslda,newdata=X[-train,])$class
> tab <- table(grp[-train],pred)
```



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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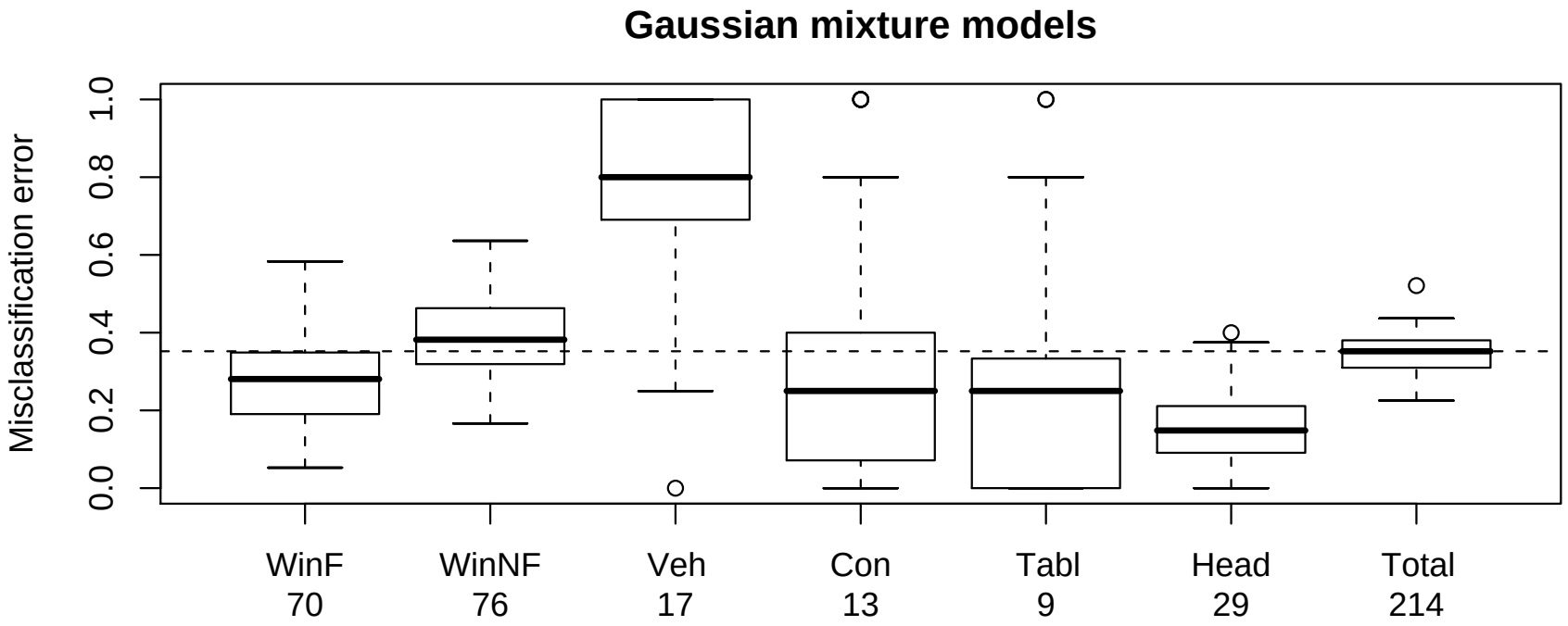
Mix: Gaussian Mixture Models

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

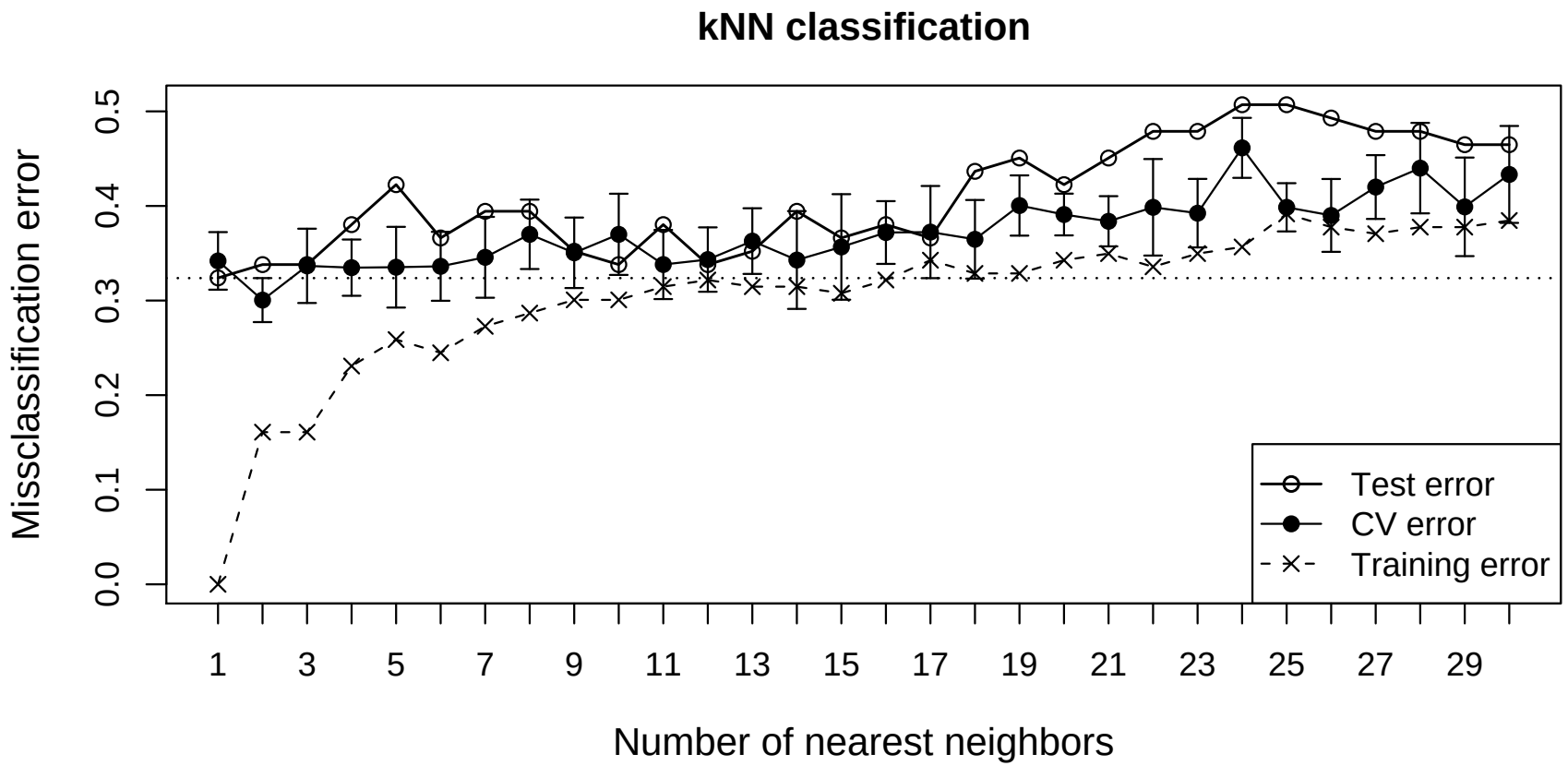
```
> train <- sample(1:n,ntrain)
> resgmm <- mda(grp ~ .,data=dat[train,])
> predgmm <- predict(resgmm,dat[-train,],type="post")
> predgrp <- apply(predgmm,1,which.max)
> tab <- table(grp[-train],predgrp)
```



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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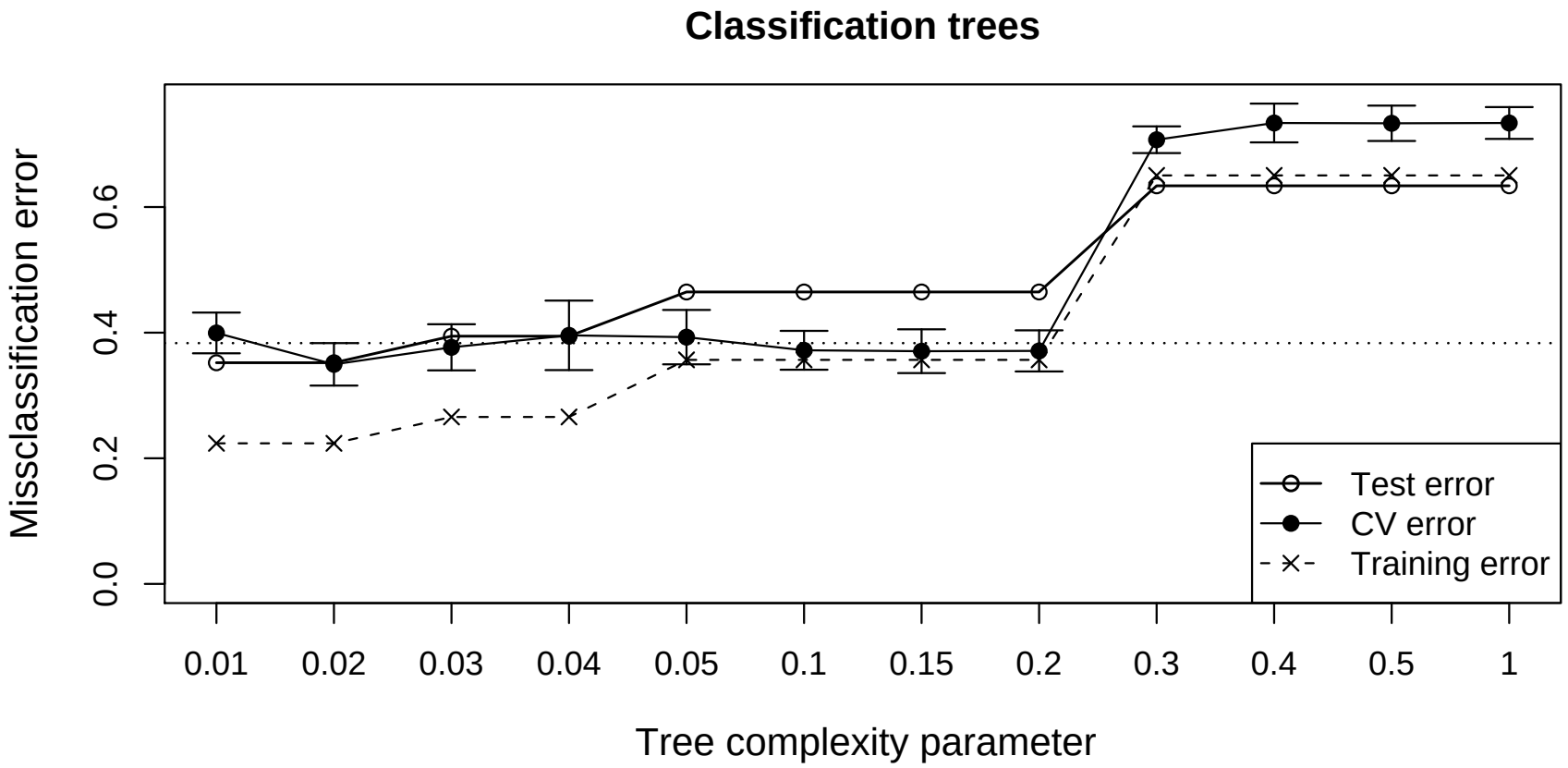
Tree: classification trees

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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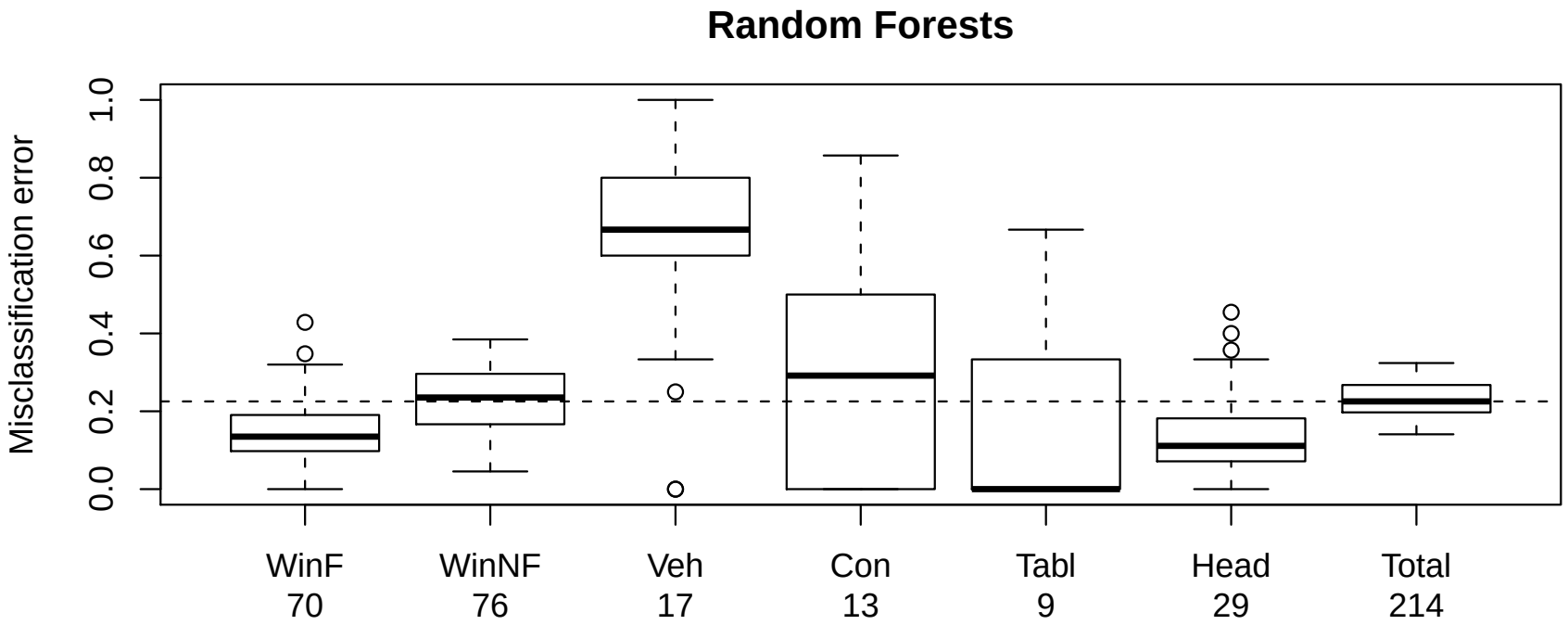
RF: Random Forests

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

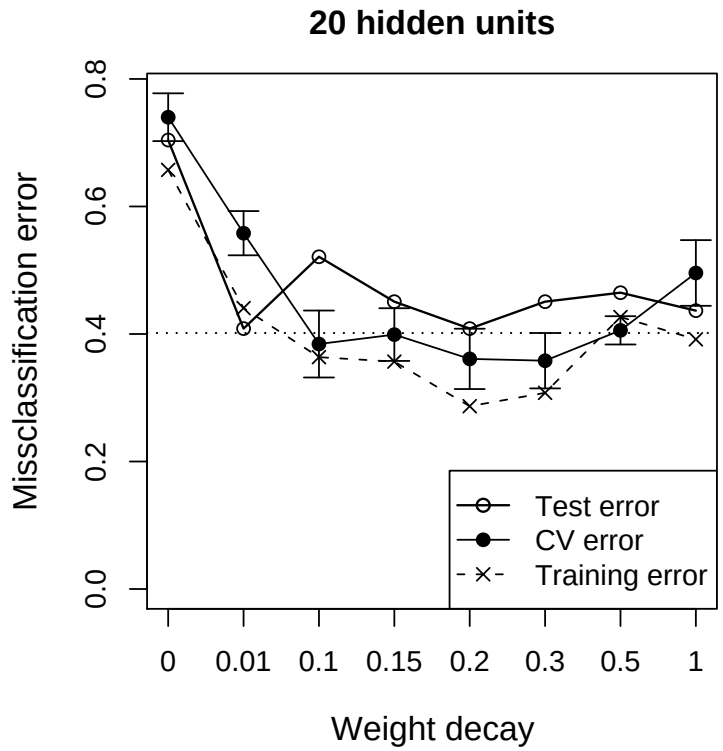
```
> train <- sample(1:n,ntrain)
> resRF <- randomForest(grp~.,data=dat,subset=train)
> predRF <- predict(resRF, dat[-train,])
> table(grp[-train],predRF)
```

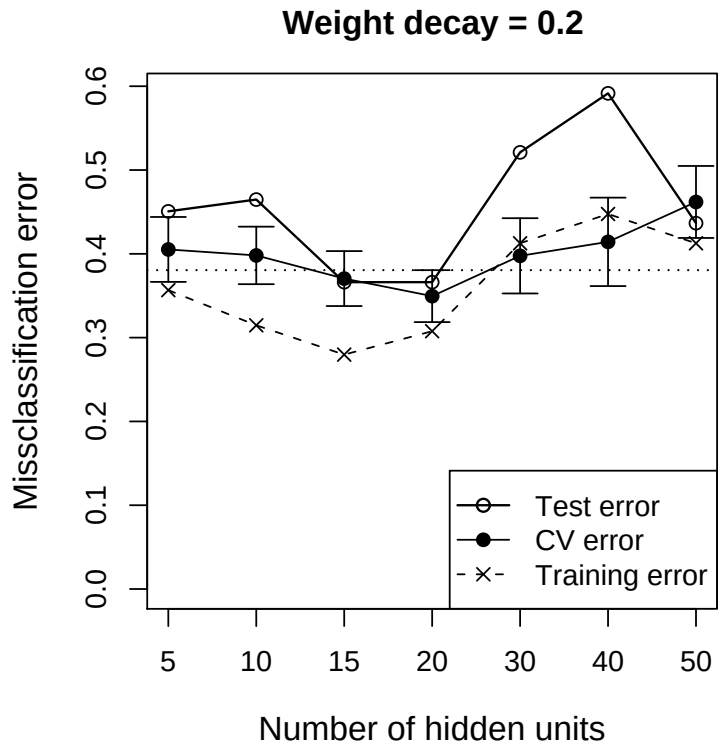


ANN: Artifician Neural Networks

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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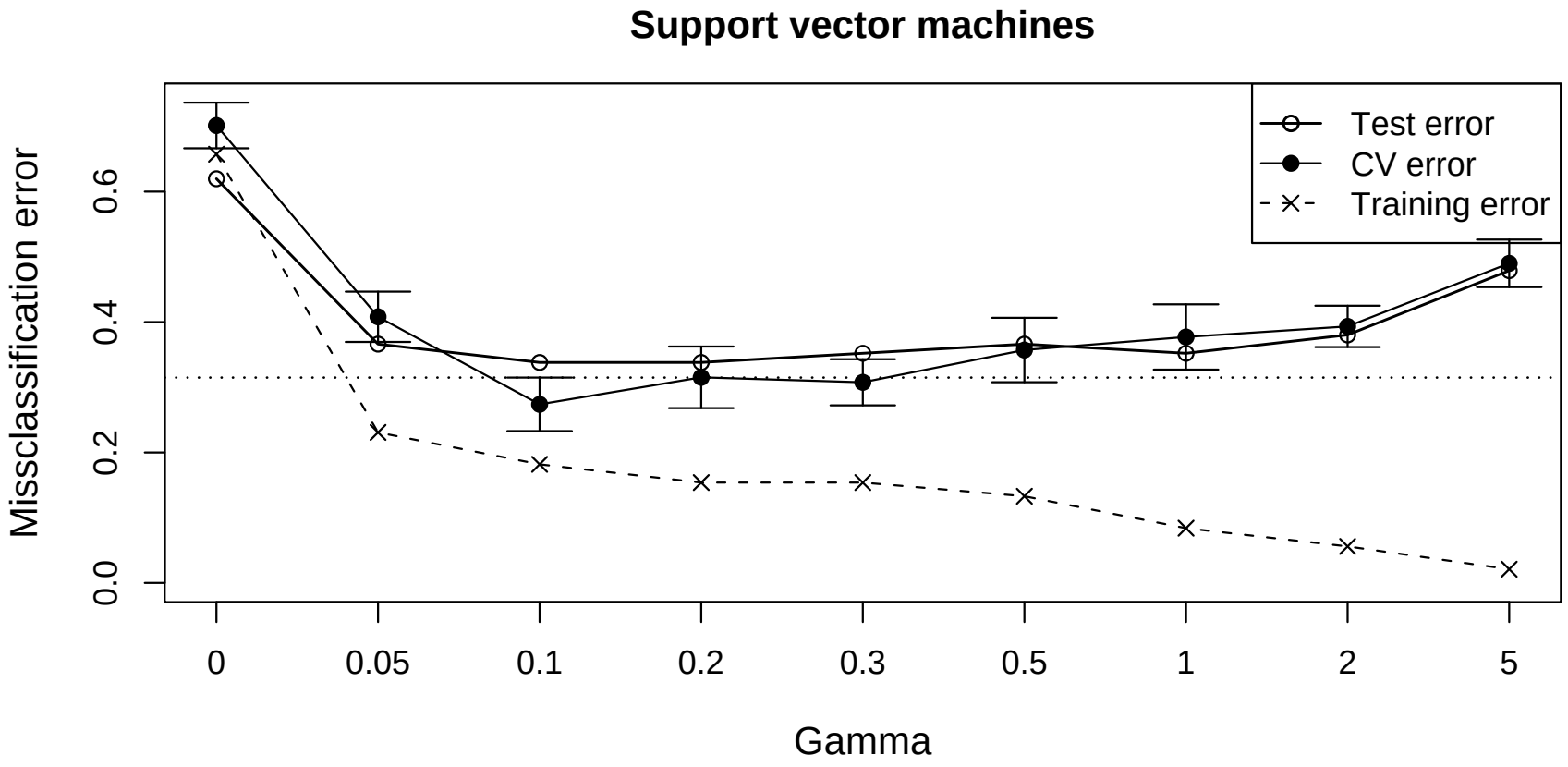
SVM: Support Vector Machines

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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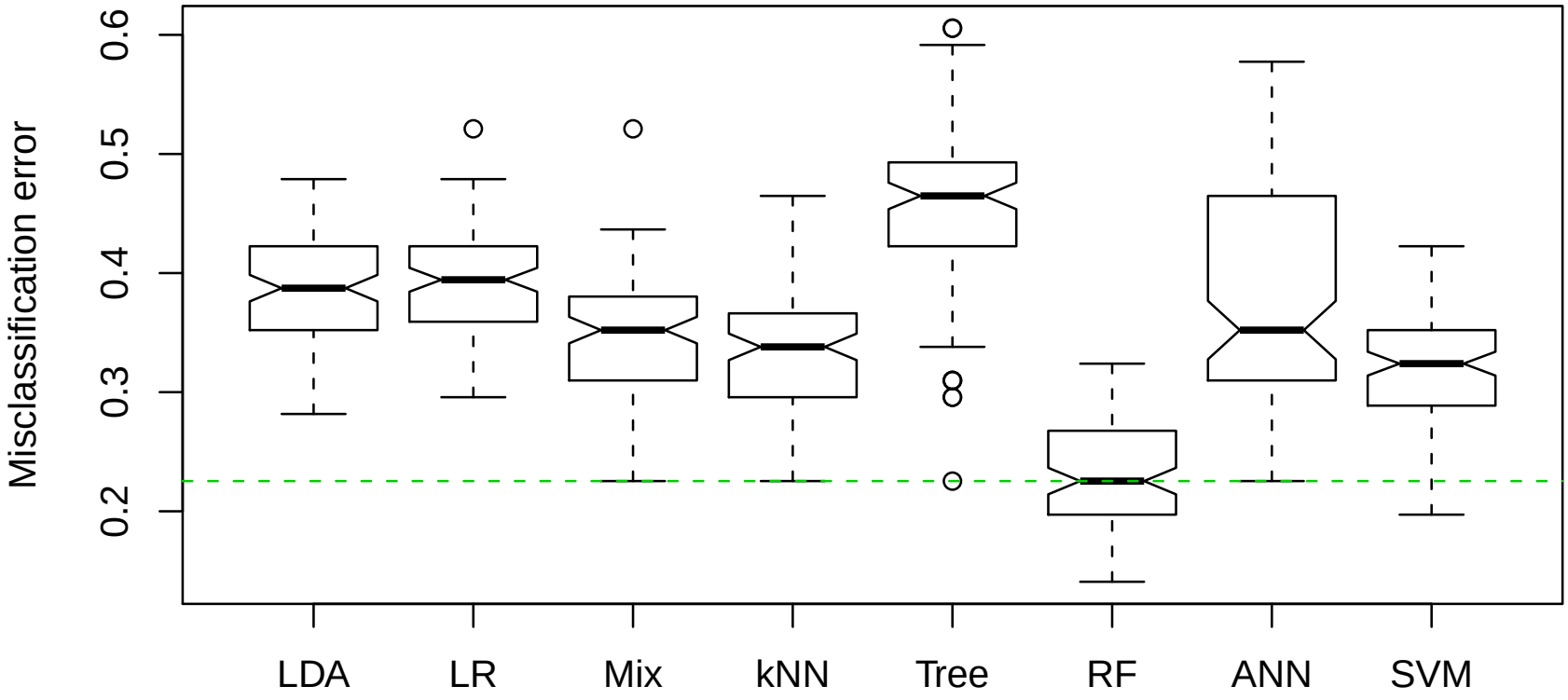
Overall Comparison



Random Forests often work surprisingly well!

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Conclusions

- **Multivariate calibration and classification:** many algorithms are available in R – the code is always "quite" similar

  In the **chemometrics** library we tried to **unify** the code and the evaluation procedures.

- **Evaluation:** should be done carefully, but *not* only for one specific method

- **Computation time:** careful evaluation requires more time–at least for larger data sets (data collection also needs time)

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