Variable Selection for Multivariate Models

Myth and Reality

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Variable Selection
for Empirical Multivariate Models

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Performance measure for calibration (rdCV method)

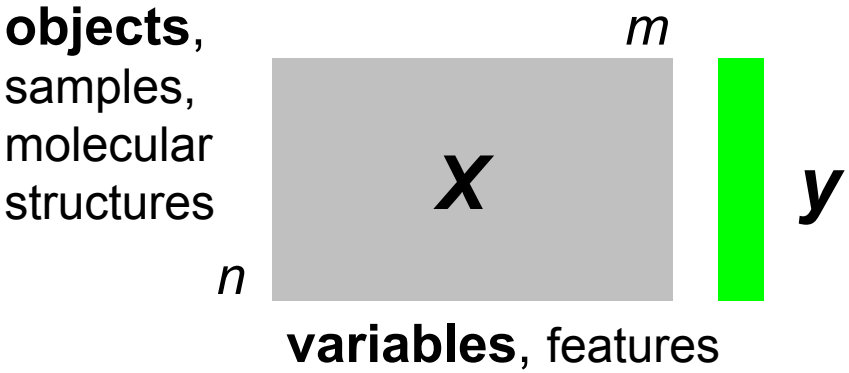
Variable selection strategy

Variable selection methods (basics, applications)

Summary

Introduction

Empirical mathematical models in chemistry



Multivariate Calibration

Linear model $\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_m x_m$

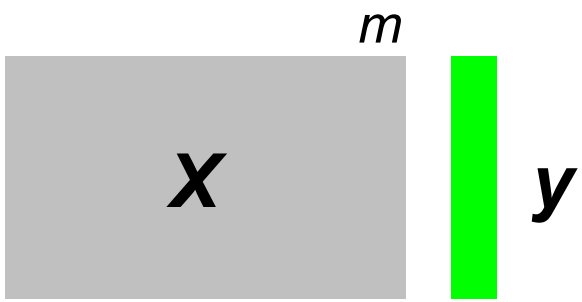
Model parameter — estimated (empirically, data driven),
e. g., by PLS regression, from a calibration set,
including optimization of model complexity

Model performance — carefully estimated for "new cases" (from a test set),
appropriate performance measure,
realistic estimation, including the variability,
requires an appropriate strategy

Introduction

Empirical mathematical models in chemistry

objects, samples, molecular structures



variables, features

desired **property**

Multivariate Calibration

Linear model $\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_m x_m$

Typical m = 10 ... several 1000 no. of variables
("all available" from instruments or software)

Variable selection Better model using only a subset of variables ($m_{SEL} << m$) ?!

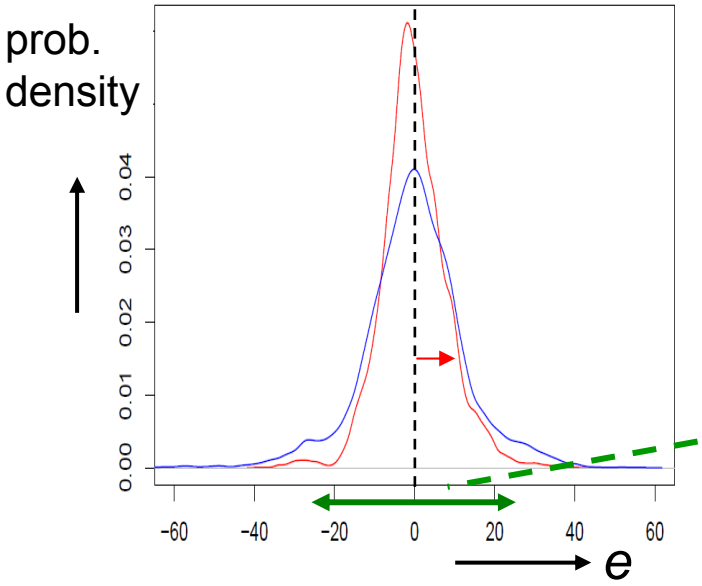
- Methods for variable selection
- Strategy for comparing model performances

Performance measure for calibration

y_i	reference ("true") value for object *i*
$\hat{y}_i$	calculated (predicted) value (test set !)
$e_i = y_i - \hat{y}_i$	prediction error for object (residual)
$i = 1 \ldots z$	*z* is the number of predictions

Specify: ☞ which data set (calibration set, **test set**)
☞ which strategy (cross validation, ...)

Distribution of prediction errors



bias = mean of prediction errors e_i

SEP = standard deviation of prediction errors e_i
= **S**tandard **E**rror of **P**rediction

SEC = **S**tandard **E**rror of **C**alibration

CI = confidence interval, $CI_{95\%} \approx \pm 2*SEP$

User friendly ! All in units of *y* !

Strategy for estimation of SEP

- **SEP has to be estimated from test set objects, not used for creation/optimization of the model**
- **SEP is not a single value but has a distribution, (estimation of the variability of SEP is essential for comparisons of SEP values)**
- **Optimum complexity of models (e. g., no. of PLS components) has to be estimated**

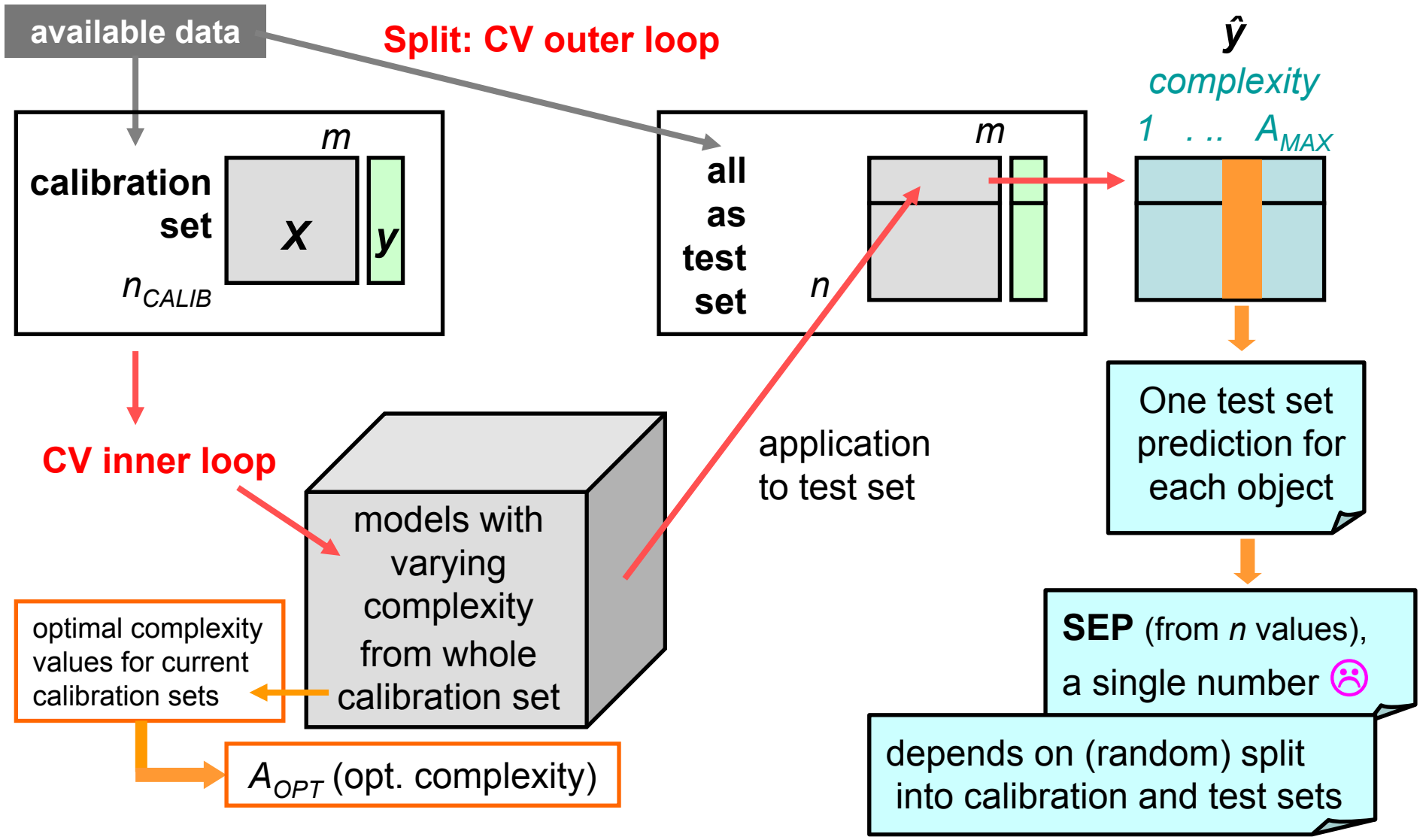
Our strategy is

repeated double Cross Validation (rdCV)

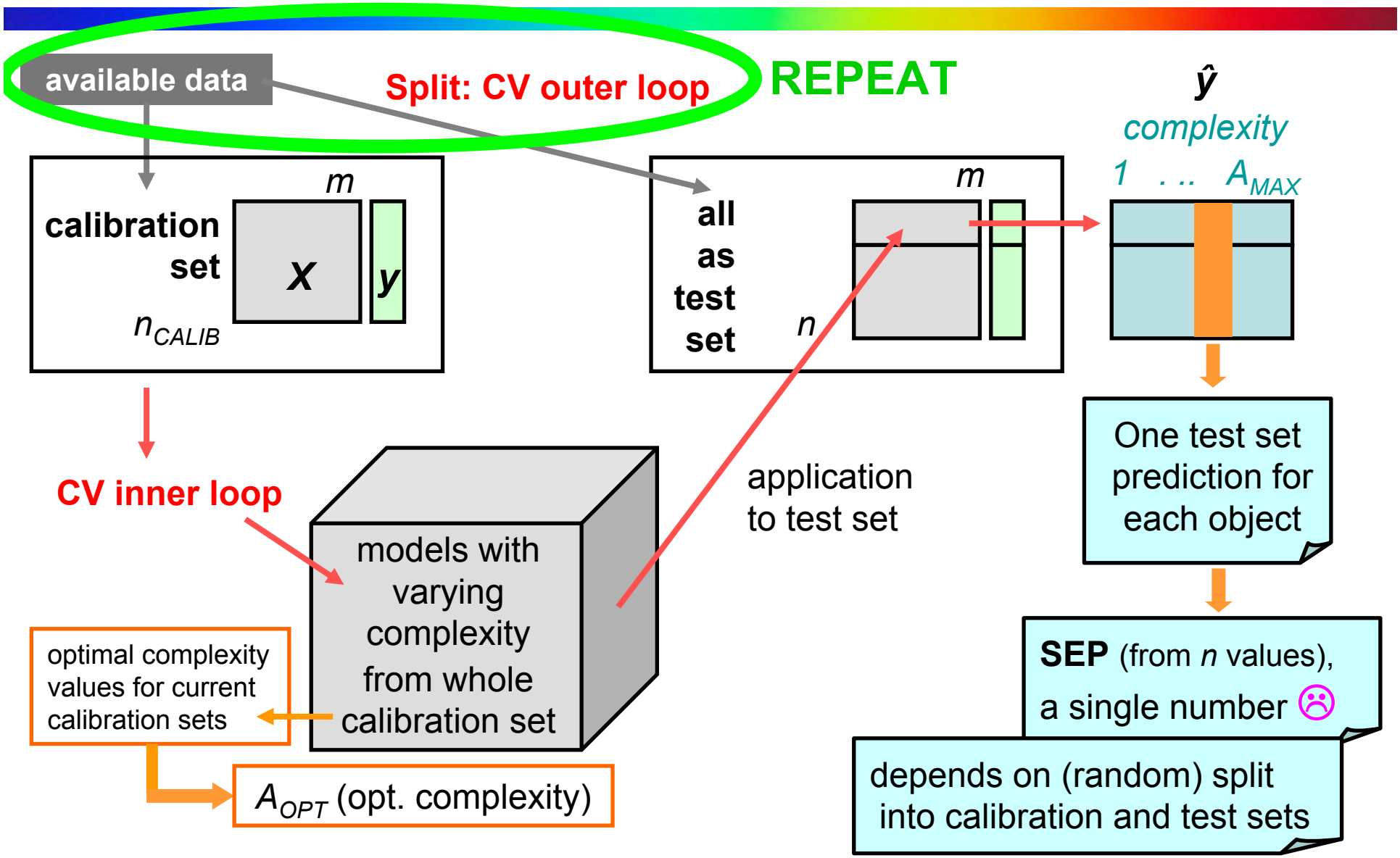
P. Filzmoser, B. Liebmann, K. Varmuza, J. Chemometrics 23 (2009) 160-171.
K. Varmuza et al., R software for chemometrics, www.lcm.tuwien.ac.at/R/

Other approaches of ***resampling***: *double bootstrap*, etc.

Strategy for estimation of SEP (rdCV)

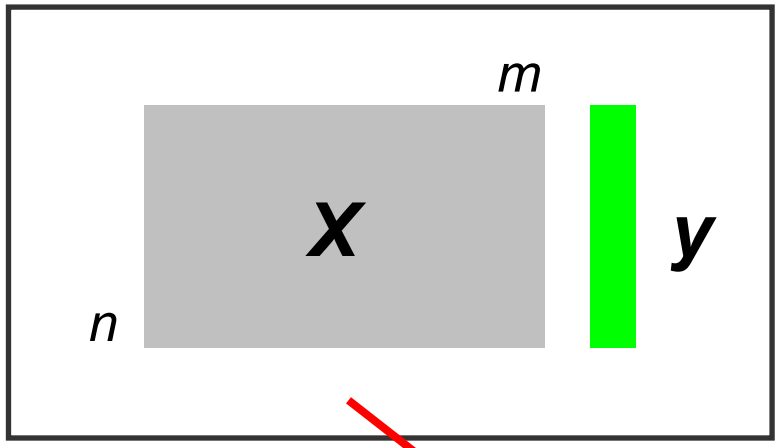


Strategy for estimation of SEP (rdCV)



Strategy for estimation of SEP (rdCV result)

available data

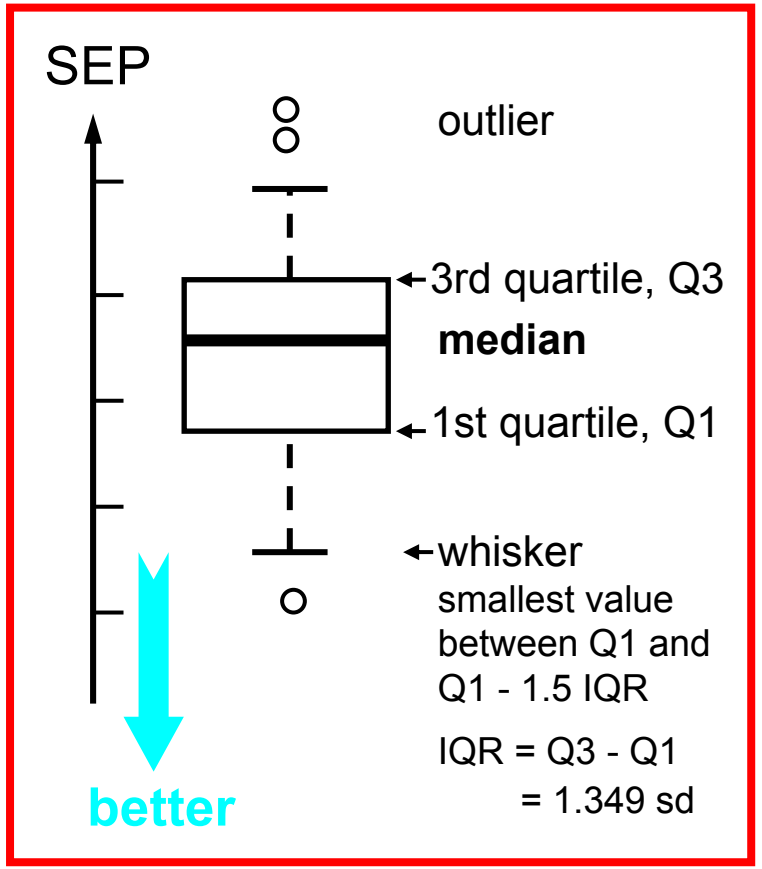


rdCV

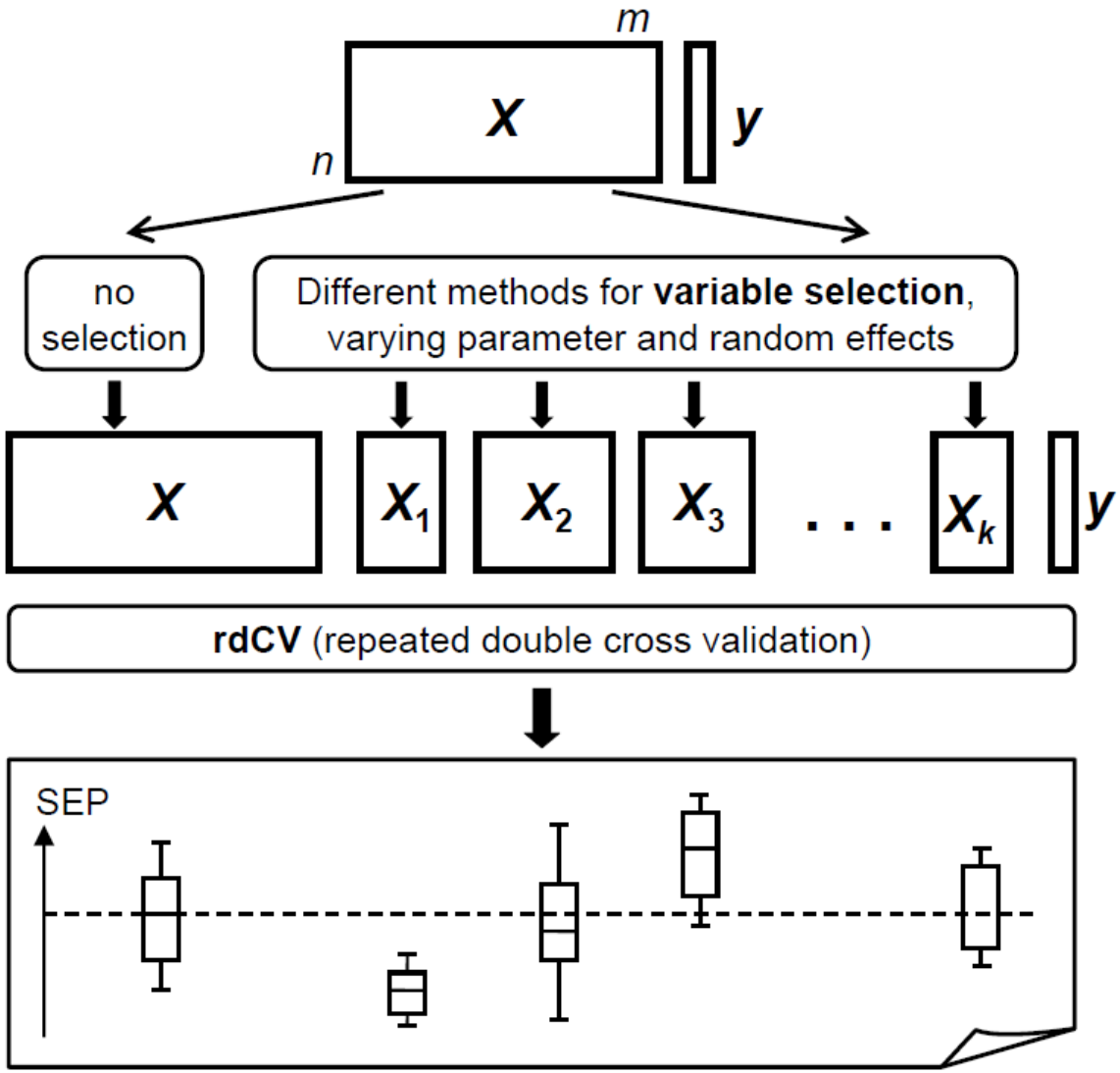
typ.: *rep* = 20 ... 100 repetitions

rep values for SEP

Characterization of the performance of models from a given data set ***X***, ***y*** by a boxplot for SEP



Variable selection / evaluation strategy



Variable selection / evaluation strategy

Performance criteria used during variable selection:

- *prediction performance for test set objects, using optimized models, would be desirable (rdCV-PLS);*

- *however, rarely applicable because too time consuming (e. g., GA may require to test several 100,000 variable sets).*

- *Most often, fit criteria are used (quick and dirty); e. g., SEP from leave-1-out, sum of squared prediction errors (within calibration set), BIC, AIC, Mallows Cp (NOT final estimations of model performance !).*

- *Therefore, evaluate suggested variable subsets carefully (goal-oriented = prediction of new cases), e. g., by rdCV (or double bootstrap).*

Variable Selection / why ?

PLS **OK** with

- $m > n$, $m >> n$
- highly correlating variables
- optimization of model complexity

- better model performance*
- interpretation of model parameter *easier*
- elimination of noise variables, more stable model parameter, *parsimony principle*

* Checked cautiously for test set objects (rdCV, bootstrap, ...).

* Not using performance measures obtained during variable selection as final model performance.

Variable Selection: *The (usually) impossible dream*

No "clever" strategy is possible to find the "best" subset of variables with guarantee.

"clever" **means not checking all possible sets**
"best" **means best test set prediction**

For *m* original ("all") variables, we have

$2^m - 1$ possible variable sets,

containing 1, 2, 3, ..., *m*-1, *m* variables
in all combinations.

?

Exhaustive ("not clever") search for best variable set:

Apply, e. g., rdCV-PLS to all **$2^m - 1$** variable sets !

Variable Selection: *The (usually) impossible dream*

m	$n\_subsets = 2^m - 1$
10	1 023
13	8 191
15	32 767
20	$1.0 \; 10^6$
35	$3.4 \; 10^{10}$
50	$1.1 \; 10^{15}$
100	$1.3 \; 10^{30}$
1000	$1.1 \; 10^{301}$

$m \leq 15$ exhaustive search (rdCV-PLS)

$m \leq 35$ best subset regression (fit !)

Data set (1) HEAT-ELE

n = 122	**biomass samples** from plants [1]
m = 13	**elemental composition** (C, H, N), and derived variables (cross products, logarithms, ratios)
y	higher **heating value**, HHV, calorimetric reference (± 60 kJ/kg) range 15 719 ... 25 948 kJ/kg

Model **heating value = f (element data)**

[1] A. Friedl, E. Padouvas, H. Rotter, K. Varmuza, Prediction of heating values of biomass fuel from elemental composition, *Anal. Chim. Acta* 544 (2005) 191-198.

Data set (2) GLU-NIR

n = 166	**fermentation samples** (cereals), centrifuged [2]
m = 232	**NIR** absorbances, 1115 - 2285 nm
y	**glucose** content, reference method HPLC range 0.32 ... 54.4 g/L

Model **glucose content = f (NIR absorbances)**

[2] B. Liebmann, A. Friedl, K. Varmuza, Determination of glucose and ethanol in bioethanol production by near infrared spectroscopy and chemometrics, *Anal. Chim. Acta* 642 (2009) 171-178.

Data set (3) PAC-QSPR

n = 209	**polycyclic aromatic compounds** chemical structures: 3D and all H-atoms (*Corina*)
m = 2661	**molecular descriptors** (*Dragon 6.0*)
y	**GC retention index** [3, 4], range 197.0 ... 503.9

Model **retention index = f (molecular descriptors)**

[3] M.L. Lee, D.L. Vassilaros, C.M. White, M. Novotny, Retention indices for programmed-temperature capillary-column gas chromatography of polycyclic aromatic hydrocarbons, *Anal. Chem.* 51 (1979) 768-773.

[4] K. Varmuza, P. Filzmoser, M. Dehmer, Multivariate linear QSPR/QSAR models: Rigorous evaluation of variable selection for PLS. *Computational and Structural Biotechnology Journal* 5 (2013) e201302007. Open access: http://dx.doi.org/10.5936/csbj.201302007; data and software: **www.lcm.tuwien.ac.at/R/**

Variable Selection Methods

- **all subsets** exhaustive: all 2^m-1 variable sets, evaluated by rdCV-PLS

$m \leq 15$

- best subset regression
- highest correlation with *y*
- highly correlating *x*-variables
- stepwise selection
- replacement
- genetic algorithm
- many others

Variable Selection: All subsets + rdCV-PLS

Criterion: SEP (rdCV)

Data: **HEAT-ELE** (122 × 13)

Variables		Best subsets (SEP_{FINAL} from rdCV)					
No.	Name	1 st	2 nd	3 rd	4 th	5 th	100 th
1	C						
2	H	■	■	■	■	■	■
3	N	■	■	■	■	■	■
4	C/H						■
5	C*H	■	■	■	■	■	■
6	C*C						
7	H*H						
8	N*N						
9	ln (C)					■	■
10	ln (H)	■	■			■	
11	ln (N)						
12	ln (C/H)						
13	ln (C*H)	■		■		■	■
m_{SEL}		5	4	4	3	6	6
SEP_{FINAL}		352.12	352.13	352.35	352.36	352.90	360.85
a_{FINAL}		3	3	3	3	3	4

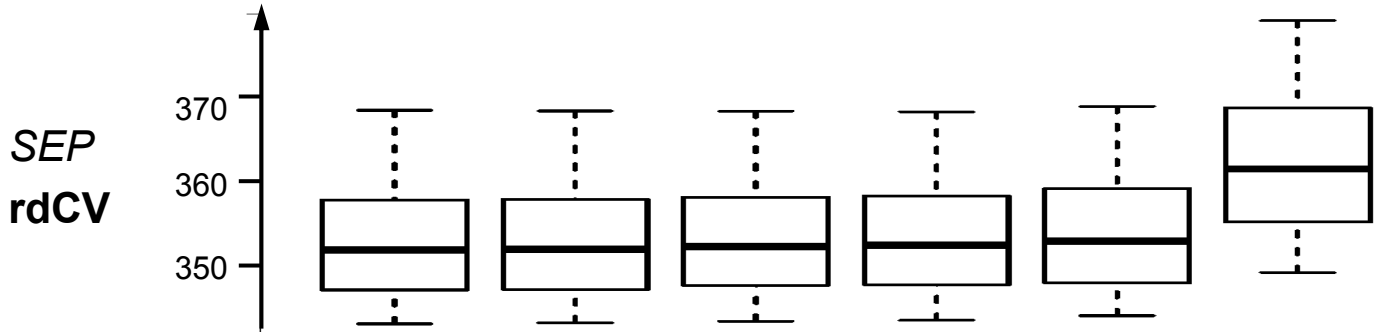
m = 13
no. of all subsets
= 2^m - 1
= 8191

↓

all subsets
tested by rdCV
(*rep* = 30, *amax* = 12
segments: 3 and 4)

↓

subsets ordered
by SEP_{FINAL}



all m = 13
variables:

SEP_{FINAL} = 417

Variable Selection: All subsets + rdCV-PLS

Criterion: SEP (rdCV)

Exhaustive and correctly evaluated.

Recommended method for
data sets with $m \leq 13$ (15) variables.

Variable Selection Methods

- all subsets
- **best subset regression**
- highest correlation with *y*
- highly correlating *x*-variables
- stepwise selection
- replacement
- genetic algorithm
- many others

variable selection optimizes fit

$m \leq 35$

Variable Selection: **Best subset regression**

Criterion: **BIC, fit criterion**

Leaps and bounds algorithm

allows an economic, complete search for subsets with a given number of variables (m_{SEL}) exhibiting best fit (BIC, etc).

Limit: ca $m \leq 35$ (although > 10^{10} subsets)

Best fit does not necessarily provide best prediction!

Therefore: **Resulting 'potentially good' subsets have to be tested for prediction performance**;

e. g., by rdCV (estimating SEP and its variability).

small BIC is fine,
value of BIC is meaningless,
just for comparisons

BIC = $n \log(RSS/n) + m \log(n)$ **B**ayes **I**nformation **C**riterion

RSS = sum of the squared residuals; log with base *e*

Variable Selection: Best subset regression

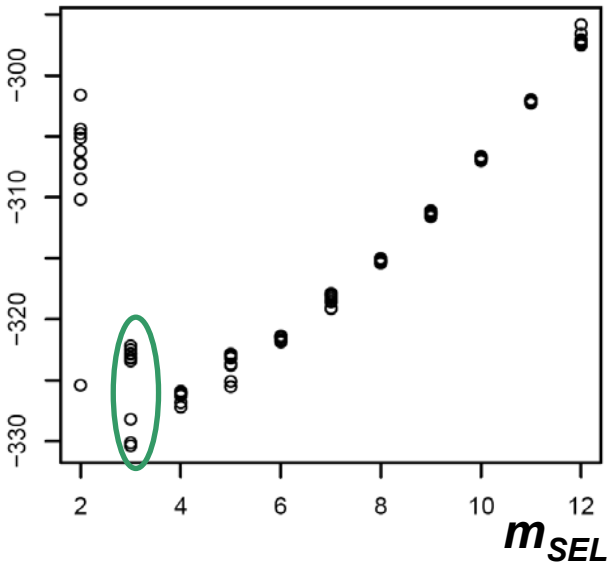
Criterion: BIC, fit criterion [R-library *leaps; regsubsets()*]

Data: **HEAT-ELE** (122 × 13)

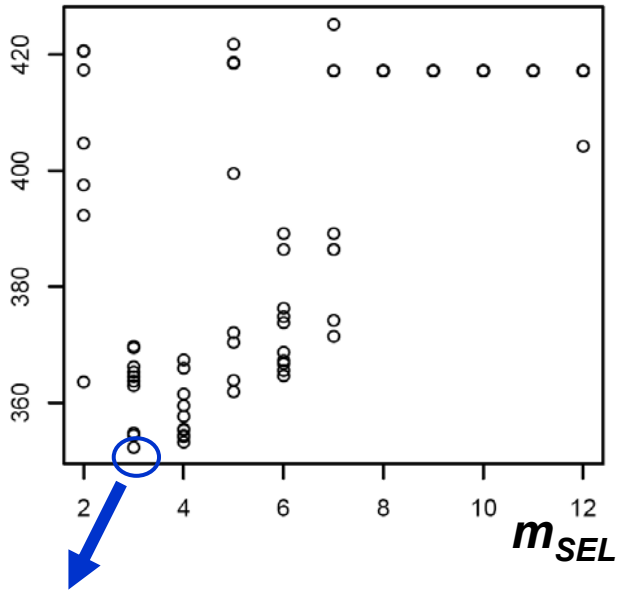
Complete search for the 10 best subsets (minimum BIC); m_{SEL} = **2 ... 12 variables**.

Estimation of prediction performance (SEP_{FINAL}) by rdCV-PLS (**110 subsets**).

BIC



SEP_{FINAL} (rdCV)



Final subset from ***best subset regression + rdCV-PLS***: m_{SEL} = 3, (H, N, C*H)

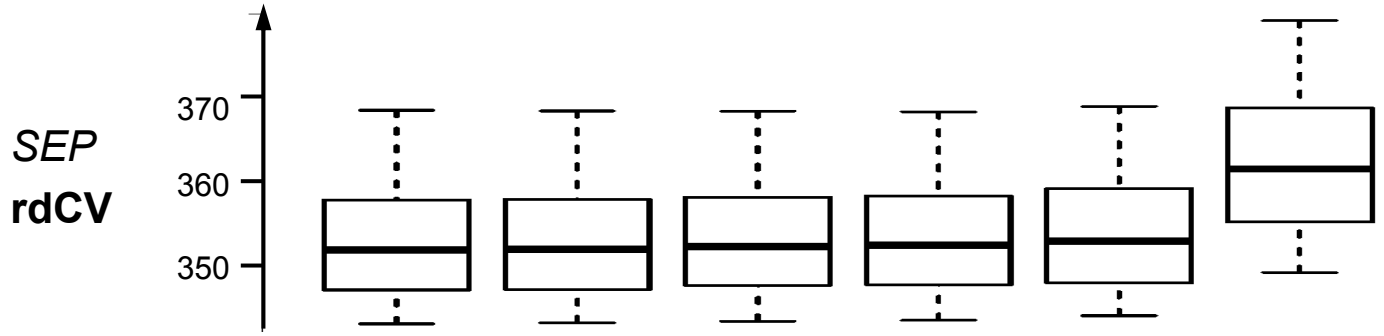
Variable Selection: All subsets + rdCV

Criterion: SEP (rdCV)

Data: **HEAT-ELE** (122 × 13)

Variables		Best subsets (SEP_{FINAL} from rdCV)					
No.	Name	1 st	2 nd	3 rd	4 th	5 th	100 th
1	C						
2	H	■	■	■	■	■	■
3	N	■	■	■	■	■	
4	C/H						
5	C*H	■	■	■	■	■	■
6	C*C						
7	H*H						
8	N*N						
9	ln (C)					■	
10	ln (H)	■	■			■	
11	ln (N)						■
12	ln (C/H)						
13	ln (C*H)	■		■		■	
m_{SEL}		5	4	4	3	6	3
SEP_{FINAL}		352.12	352.13	352.35	352.36	352.90	354.47
a_{FINAL}		3	3	3	3	3	3

Best subset regression



Variable Selection: **Best subset regression**

Criterion: **BIC, fit criterion** [R-library *leaps; regsubsets()*]

Try for datasets with $m \leq 35$ variables.

Consider several suggested variable subsets and test for prediction performance.

May give near optimum results.

Variable Selection Methods

- all subsets
- best subset regression
- **highest correlation with *y***
- **highly correlating *x*-variables**
- stepwise selection
- replacement
- genetic algorithm
- many others

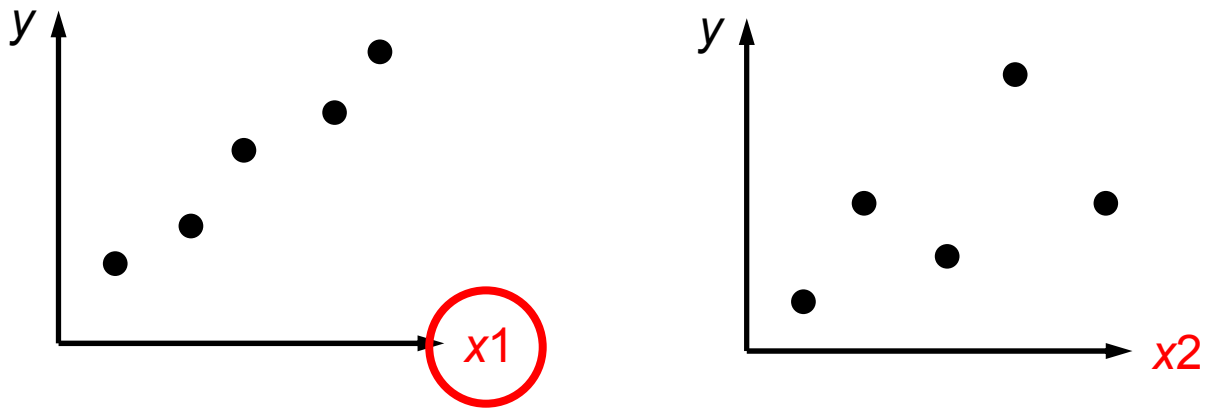
univariate,
fast, simple, evident,
for many variables

Variable Selection: corr xy

Select variables possessing highest correlation with y

Criterion: Squared (Pearson) correlation coefficient [cor(x_j, y)]^2

Linear model $\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_m x_m$



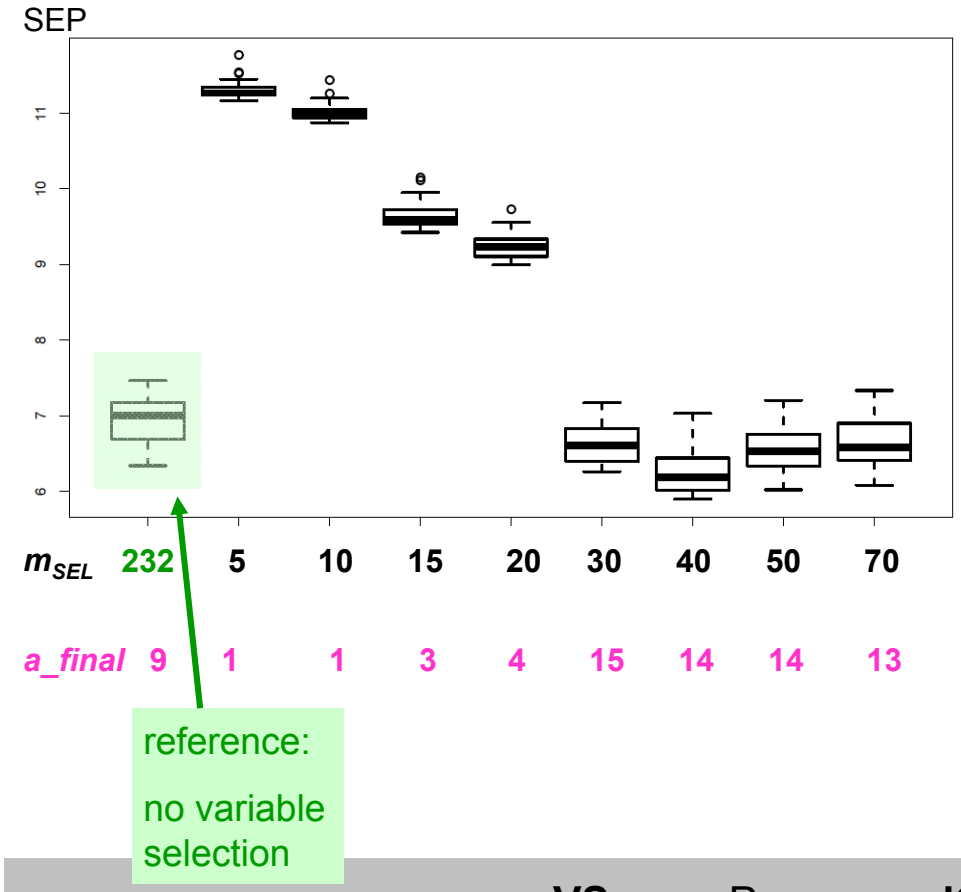
- Select a subset of variables (m_{SEL}) with maximum
  squared Pearson correlation coefficient (etc.), $R^2(x_j, y)$
- Delete variables with very low
  squared Pearson correlation coefficient (etc.), $R^2(x_j, y) <$ **threshold**

Variable Selection: corr xy

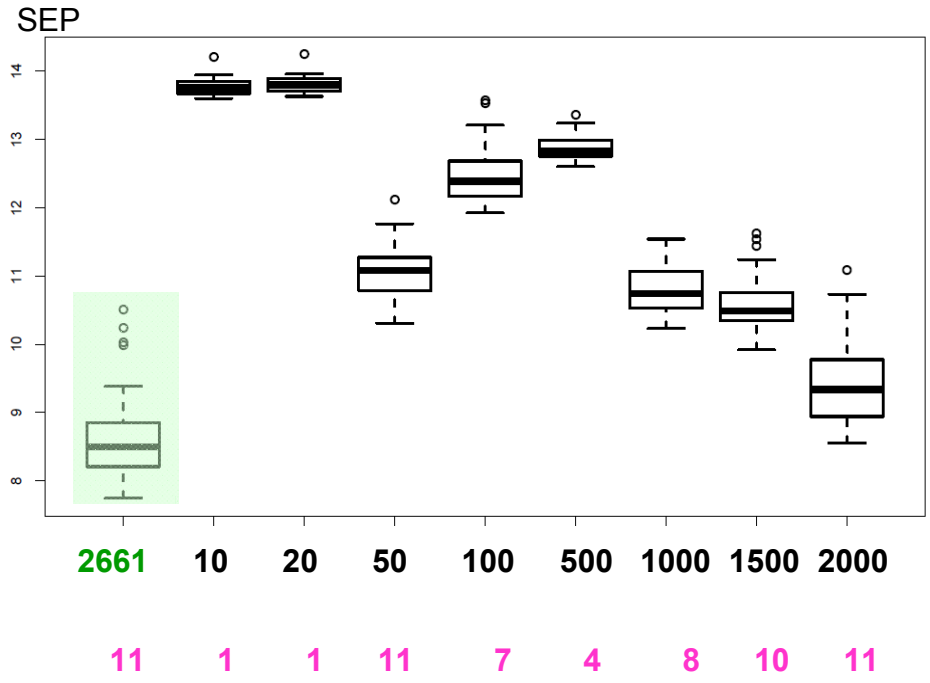
Select variables possessing highest correlation with y

Criterion: Squared (Pearson) correlation coefficient [cor(x_j, y)]^2

Data: **GLU-NIR** (166 × 232)



Data: **PAC-QSPR** (209 × 2661)



VS: squ. Pearson; **rdCV:** rep=30, amax=20

Variable Selection: corr xy

Select variables possessing highest correlation with y

Criterion: Squared (Pearson) correlation coefficient $[\text{cor}(x_j, y)]^2$

No or no significant improvement of prediction performance.

Success depends on data structure.

Variable Selection: corr xx

Eliminate variables possessing very high correlation with another variable

Criterion: Squared (Pearson) correlation coefficient [cor(x_j, x_k)]^2

Eliminate variables that are

- identical to another variable,
- have a large **squared Pearson correlation coefficient** (etc.), $R^2(x_j, x_k)$ to another variable (*), threshold e. g., 0.99, 0.95, ...

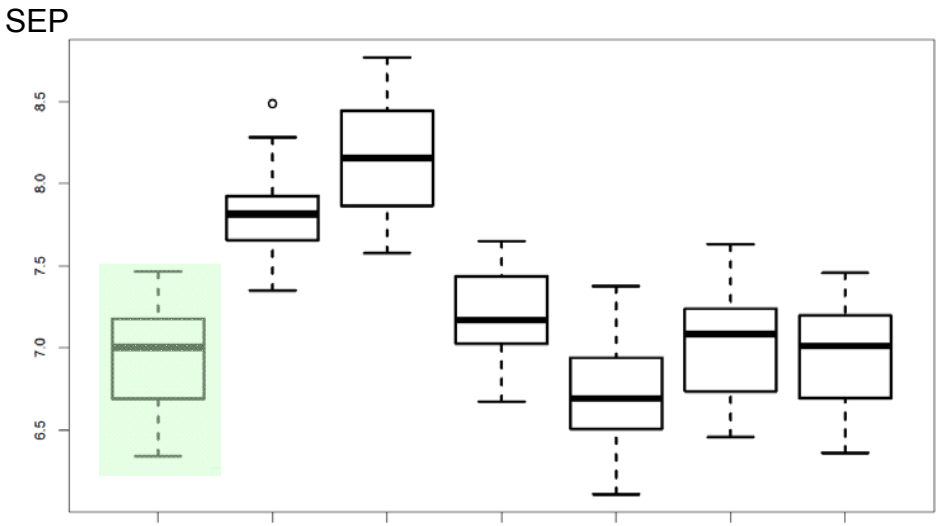
(*) Eliminate the variable with the larger sum of R^2 to all other variables.

Variable Selection: corr xx

Eliminate variables possessing very high correlation with another variable

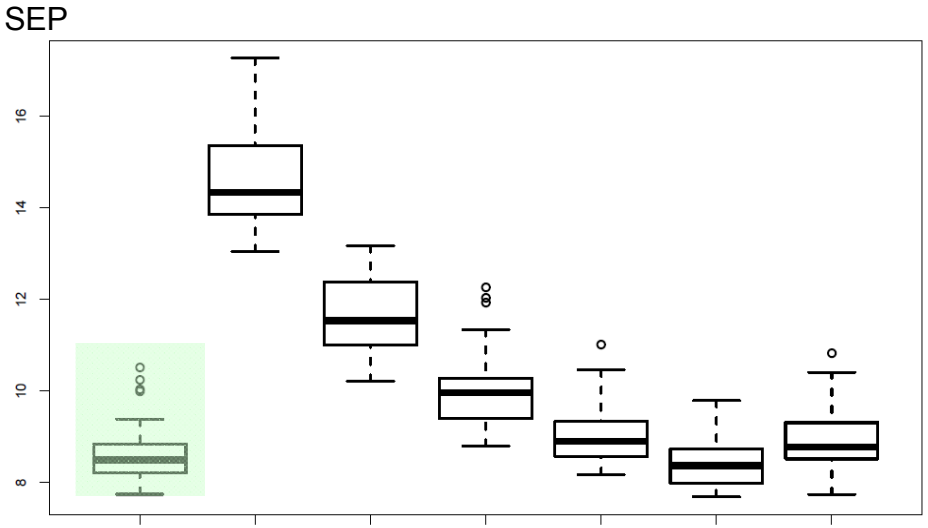
Criterion: Squared (Pearson) correlation coefficient [cor(x_j, x_k)]^2

Data: **GLU-NIR** (166 × 232)



m_{SEL}	232	15	20	42	73	173	222
R^2_{LIMIT}		0.7	0.8	0.9	0.95	0.99	0.999
a_final	9	10	10	12	12	9	9

Data: **PAC-QSPR** (209 × 2661)



m_{SEL}	2661	281	432	685	932	1474	2046
R^2_{LIMIT}		0.7	0.8	0.9	0.95	0.99	0.999
a_final	11	14	10	12	13	12	12

VS: squ. Pearson; **rdCV:** rep=30, amax=20

Variable Selection: corr xx

Eliminate variables possessing very high correlation with another variable

Criterion: Squared (Pearson) correlation coefficient $[\text{cor}(x_j, x_k)]^2$

No improvement of prediction performance.

Elimination of variables with $R^2(x_j, x_k) > 0.99$ does not decrease the prediction performance.

Success depends on data structure.

Variable Selection Methods

- all subsets
- best subset regression
- highest correlation with *y*
- highly correlating *x*-variables
- **stepwise selection**
- replacement
- genetic algorithm
- many others

- start with one variable (or with all variables),
- add/delete single variables ("step"),
- standard method,
- best fit,
- applicable for many variables

Variable Selection: stepwise

Criterion: BIC

"Forward" stepwise selection: starts with an "empty model" (*y* is explained only by the intercept), and adds in each step one variable (the "best") until no further improvement is possible.

"Backward" stepwise selection: starts with the "full model" (all x-variables; not possible if e.g., $m > n$), and removes in each step one variable (the "worst") until no further improvement is possible.

"Both" directions stepwise selection: adding or removing one variable at a time, starting either from the empty (!) or from the full model until no further improvement is possible.

BIC can be used instead of the more traditional F-test

Variable Selection: stepwise

Criterion: BIC

New R function: varsel_stepwise_BIC()

Peter Filzmoser, TU Vienna

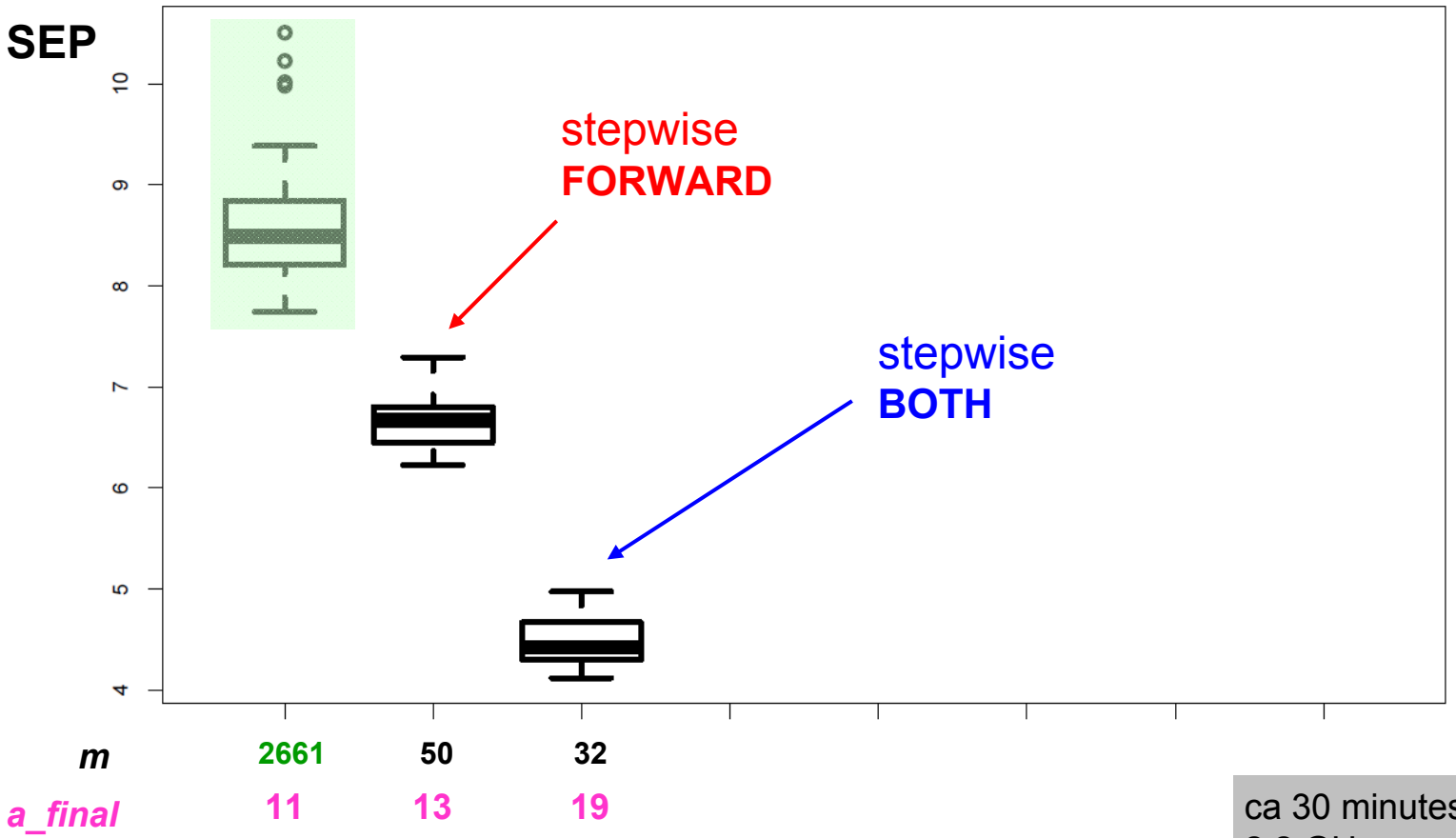
- "Forward" or "Both" strategy.
- Stop until no more improvement (BIC), or until a certain number of steps, or a pre-defined computing time is reached.
- Much faster (for e. g., $m > 100$) than the long existing R function **step()**.
- Still time consuming for $m > 1000$.

Free download: www.lcm.tuwien.ac.at/R/

Variable Selection: stepwise

Criterion: BIC

Data: **PAC-QSPR** (209 × 2661)



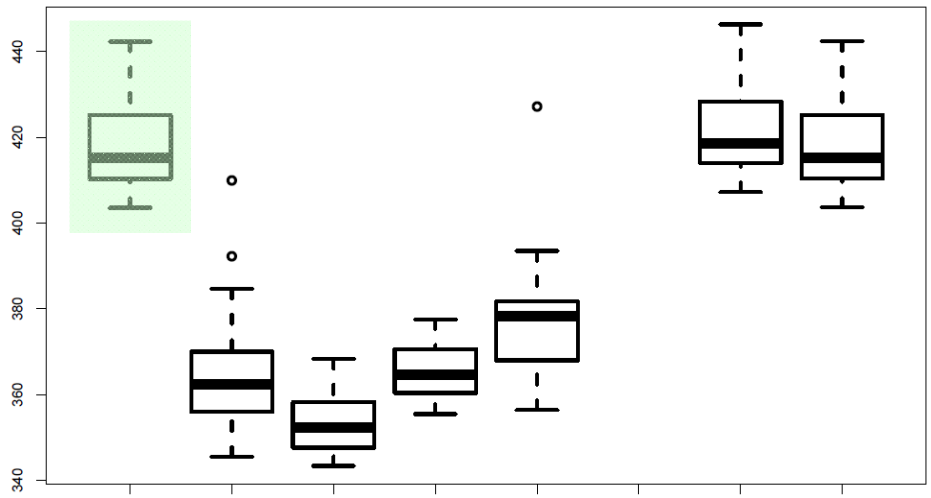
ca 30 minutes
2.2 GHz

VS: BIC, max 50 steps; **rdCV:** rep=30, amax=20

Variable Selection: stepwise

Criterion: BIC

Data: **HEAT-ELE** (122 × 13)



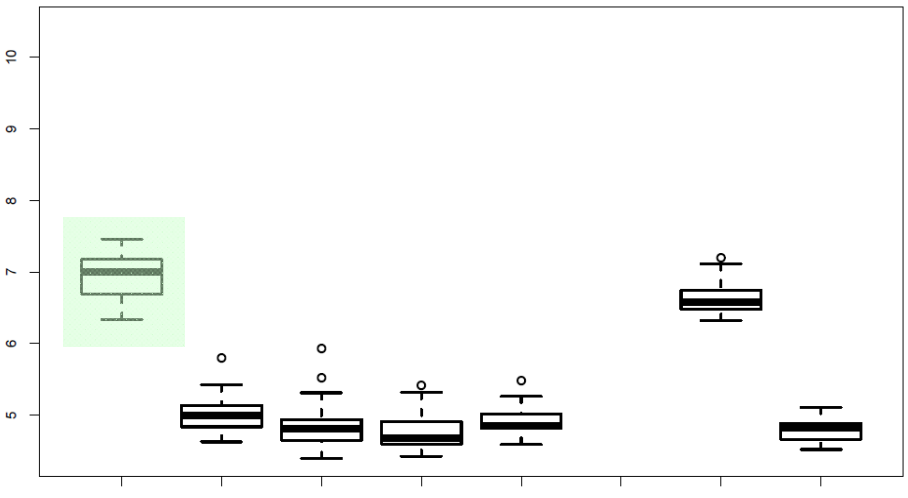
m	13	5	3	2	3	2	4	
a_final	1	4	3	2	3	1	1	

stepwise **FWD | BOTH**

corr xy **(>0.1 | >0.2)** stepwise **BOTH**

corr xx **(<0.95 | <0.99)** stepwise **BOTH**

Data: **GLU-NIR** (166 × 232)



m	232	16	16	15	15	10	15	
a_final	9	13	14	9	13	7	14	

stepwise **FWD | BOTH**

corr xy **(>0.1 | >0.2)** stepwise **BOTH**

corr xx **(<0.95 | <0.99)** stepwise **BOTH**

VS: BIC, squ. Pearson (x, y) or (x, x), max 50 steps; **rdCV:** rep=30, amax=12 or 20

Variable Selection: stepwise

Criterion: BIC

Significant improvement of prediction performance.

Strategy *BOTH* (starting *FORWARD*) is often best.

Computing time	**ca 20 s**	**for $m = 200$**
	ca 20 min	**for $m = 2000$**

Variable Selection Methods

- all subsets
- best subset regression
- highest correlation with *y*
- highly correlating *x*-variables
- stepwise selection
- **replacement**
- genetic algorithm
- many others

- **sequential replacement**
- start with randomly selected m_{SEL} variables
- replace single variables ("step"),
- rarely used,
- best fit

Variable Selection: Sequential replacement

Criterion (fitness): BIC, fit criterion [R-library *leaps; regsubsets()*]

Start with a random set of m_{SEL} variables.

Replace each variable with one of the not selected variables - and keep a new variable if it improves the model performance.

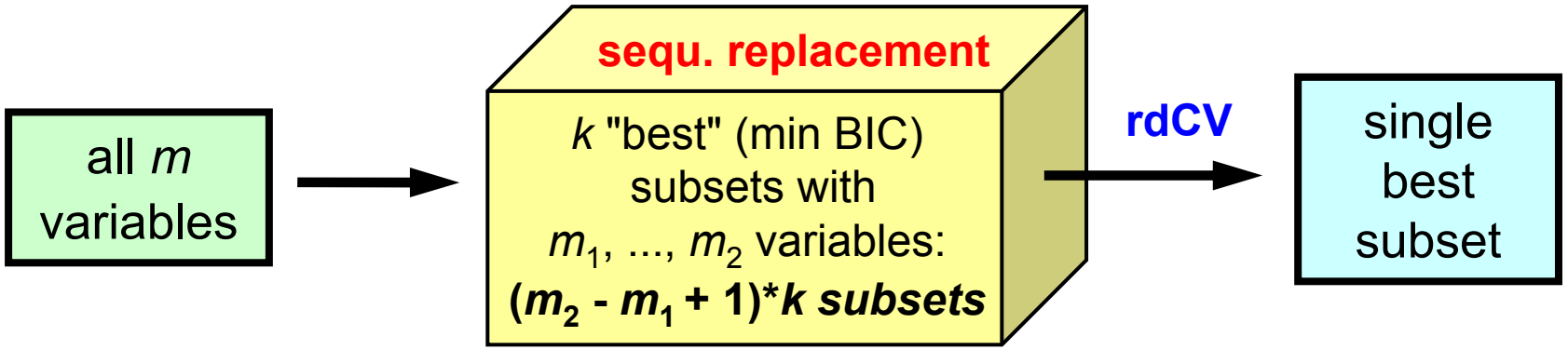
Repeat this procedure until the variable subset is stable or a terminating criterion is reached.

Miller A.: Subset Selection in Regression, 2nd ed., Chapman & Hall - CRC (2002). [1st ed. 1990]

Mercader A.C., Castro E.A.: in Statistical Modelling of Molecular Descriptors in QSAR/QSPR, p. 149, ed. Dehmer M., Varmuza K., Bonchev D., Wiley-VCH, Weinheim (2012).

Todeschini R., et. al.: Reshaped sequential replacement for variable selection (2013).

Our strategy



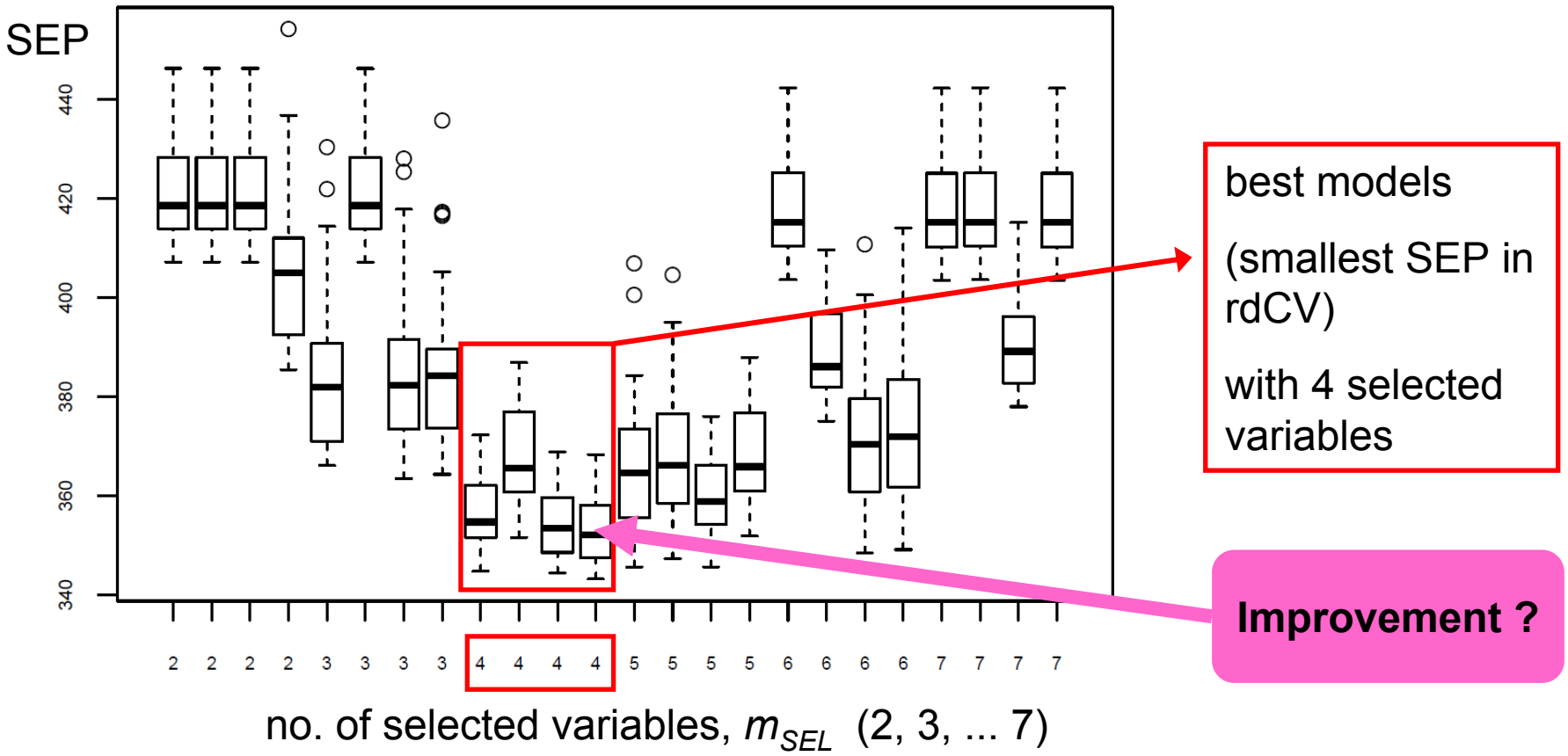
Variable Selection: Sequential replacement

Criterion (fitness): BIC, fit criterion [R-library *leaps; regsubsets()*]

Data: **HEAT-ELE** (122 × 13)

(1) Search **best 4** subsets containing **2 ... 7 variables**: (7-2+1)*4 = **24 subsets**

(2) Evaluate these 24 subsets by rdCV



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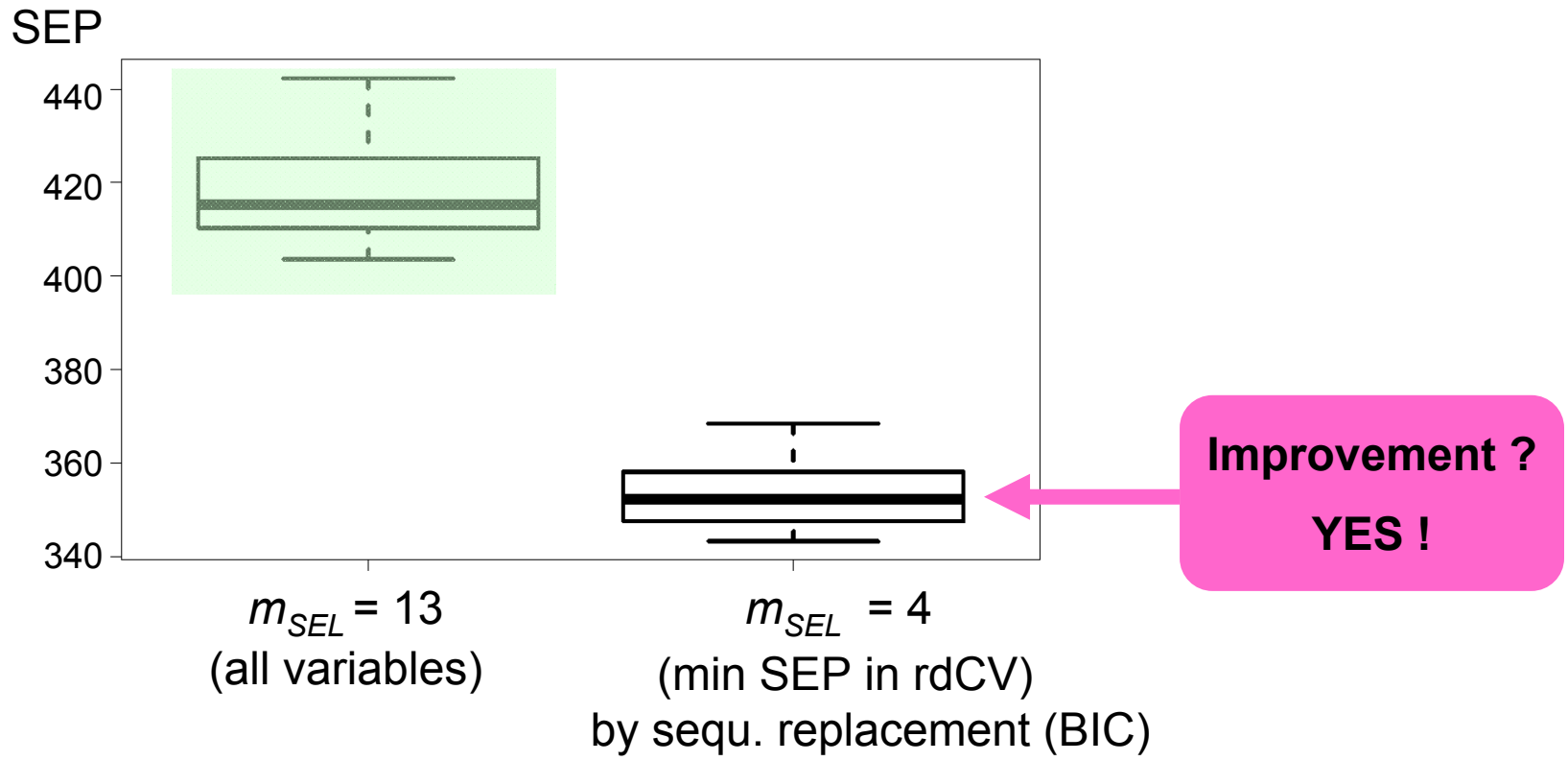


Variable Selection: All subsets + rdCV

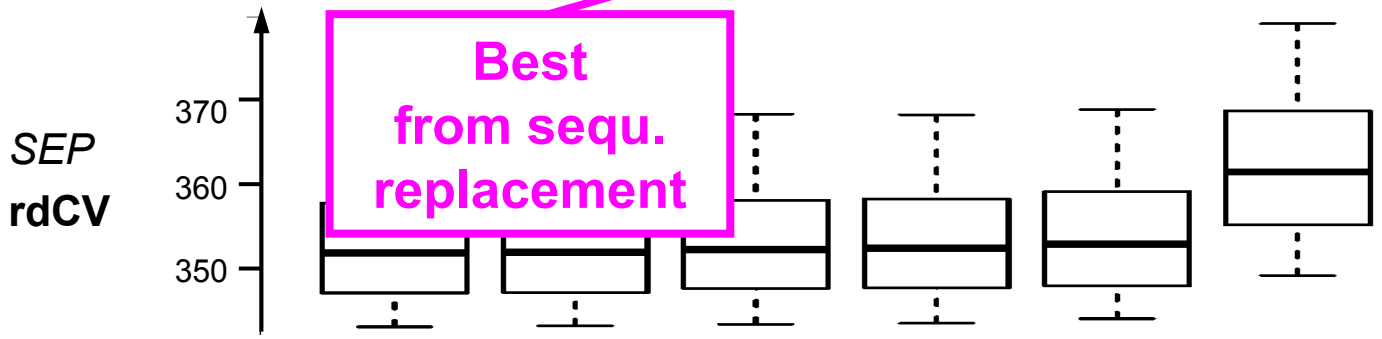
Criterion: SEP (rdCV)

Data: **HEAT-ELE** (122 × 13)

Variables		Best subsets (SEP_{FINAL} from rdCV)					
No.	Name	1 st	2 nd	3 rd	4 th	5 th	**20 th**
1	C						
2	H	■	■	■	■	■	■
3	N	■	■	■	■	■	
4	C/H						
5	C*H	■	■	■	■	■	■
6	C*C						
7	H*H						
8	N*N						
9	ln (C)					■	
10	ln (H)	■	■			■	
11	ln (N)						■
12	ln (C/H)						
13	ln (C*H)	■		■		■	
m_{SEL}		**5**	**4**	**4**	**3**	**6**	**3**
SEP_{FINAL}		**352.12**	**352.13**	**352.35**	**352.36**	**352.90**	**354.47**
a_{FINAL}		3	3	3	3	3	**3**

Best subset regression

Best from sequ. replacement



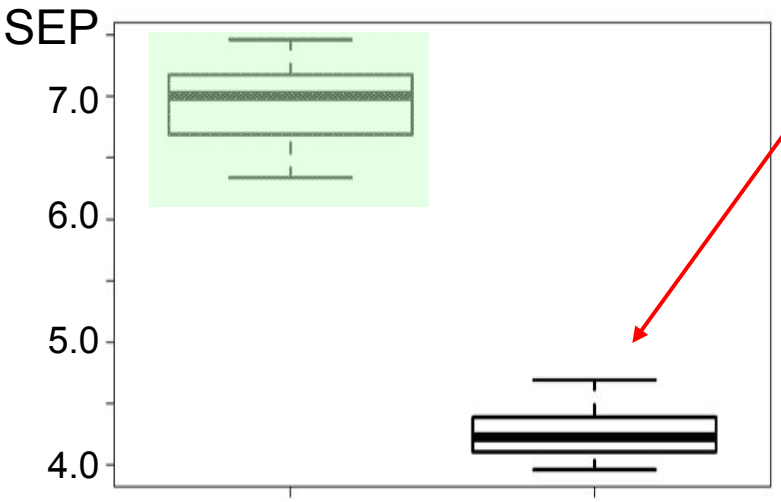
Variable Selection: Sequential replacement

Criterion (fitness): BIC, fit criterion [R-library *leaps; regsubsets()*]

Data: **GLU-NIR** (166 × 232)

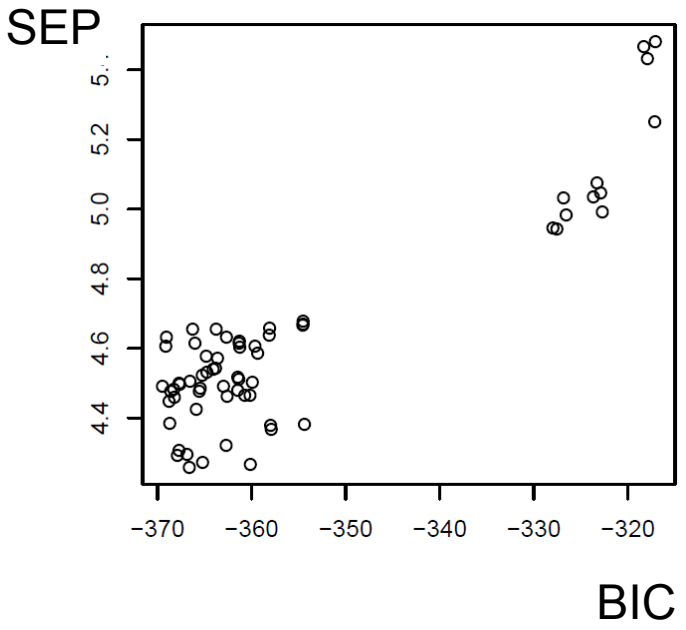
(1) Search **best 4** subsets containing **10 ... 25 variables**: (25-10+1)*4 = **64 subsets**

(2) Evaluate these 64 subsets by rdCV; select best (SEP)



m_{SEL} = 232
(all variables)

m_{SEL} = 20
(min SEP in rdCV)
variables selected by
sequ. replacement (BIC)



Variable Selection: Sequential replacement

Criterion (fitness): BIC, fit criterion [R-library *leaps; regsubsets()*]

Significant improvement of prediction performance.

Time consuming.

Rather not appropriate for *m* >1000.

Variable Selection Methods

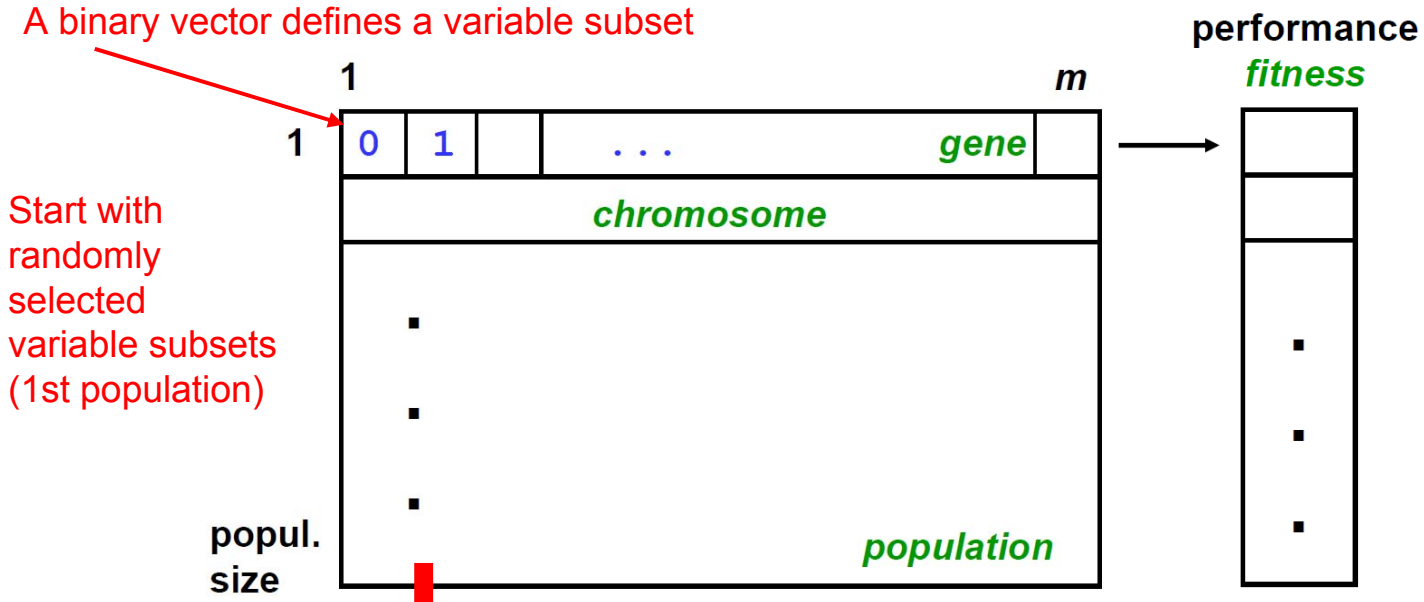
- all subsets
- best subset regression
- highest correlation with *y*
- highly correlating *x*-variables
- stepwise selection
- replacement
- **genetic algorithm**
- many others

- a *nature-inspired* method (terminology),
- search for near-optimum solutions (trying to avoid local optima, some randomness),
- time-consuming,
- rather not for many variables

Variable Selection: Genetic Algorithm (GA)

Criterion (fitness): $R^2(y, \hat{y})$ - adjusted, ...

simplified overview



Modify the population by GA strategies (*evolution, genetics,* ...) with the final aim to improve the fitness of the best variable subsets:

- eliminate worst chromosomes (*fittest survive*);
- combine best chromosomes to a new one (e. g., *cross-over*)
- random modifications of genes (*mutations*)
- consider defined restrictions, ...

Estimate fitness for new variable subsets (new population, a *generation*), until no improvement appears or a termination criterion is reached.

Best variable subset(s) [chromosomes] are the solution for variable selection.

Variable Selection: Genetic Algorithm (GA)

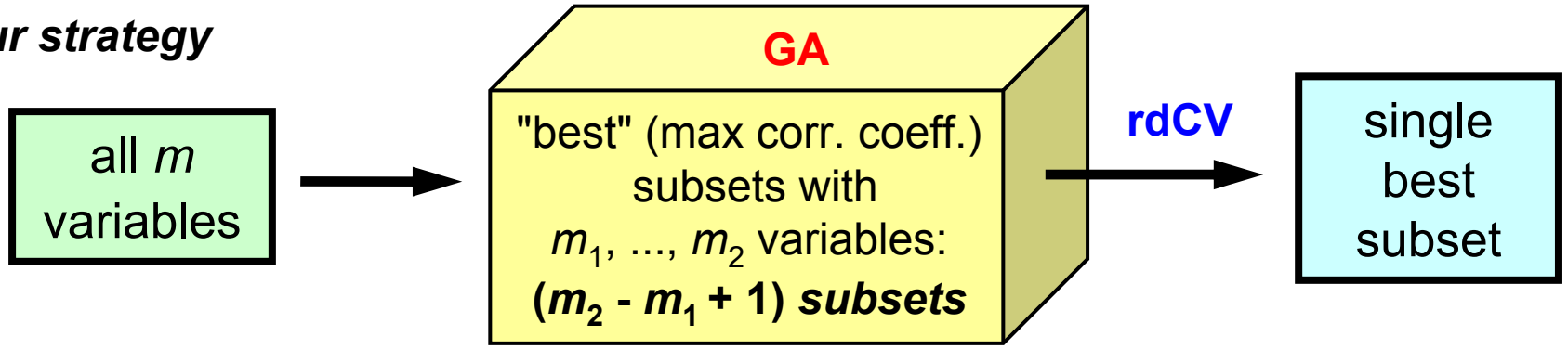
Criterion (fitness): $R^2(y, \hat{y})$, **Pearson (!)** **[R-library *subselect; genetic()*]**

Population size: $2m$ (min 100, max 500)
Stopping rule: no. of generations (typ. 500)

Result of GA: Variable subsets with highest R^2 (Pearson) containing m_{SEL} variables ($m_{SEL} = m_1 \ldots m_2$)

Careful test of the suggested variable subsets necessary (rdCV).

Our strategy

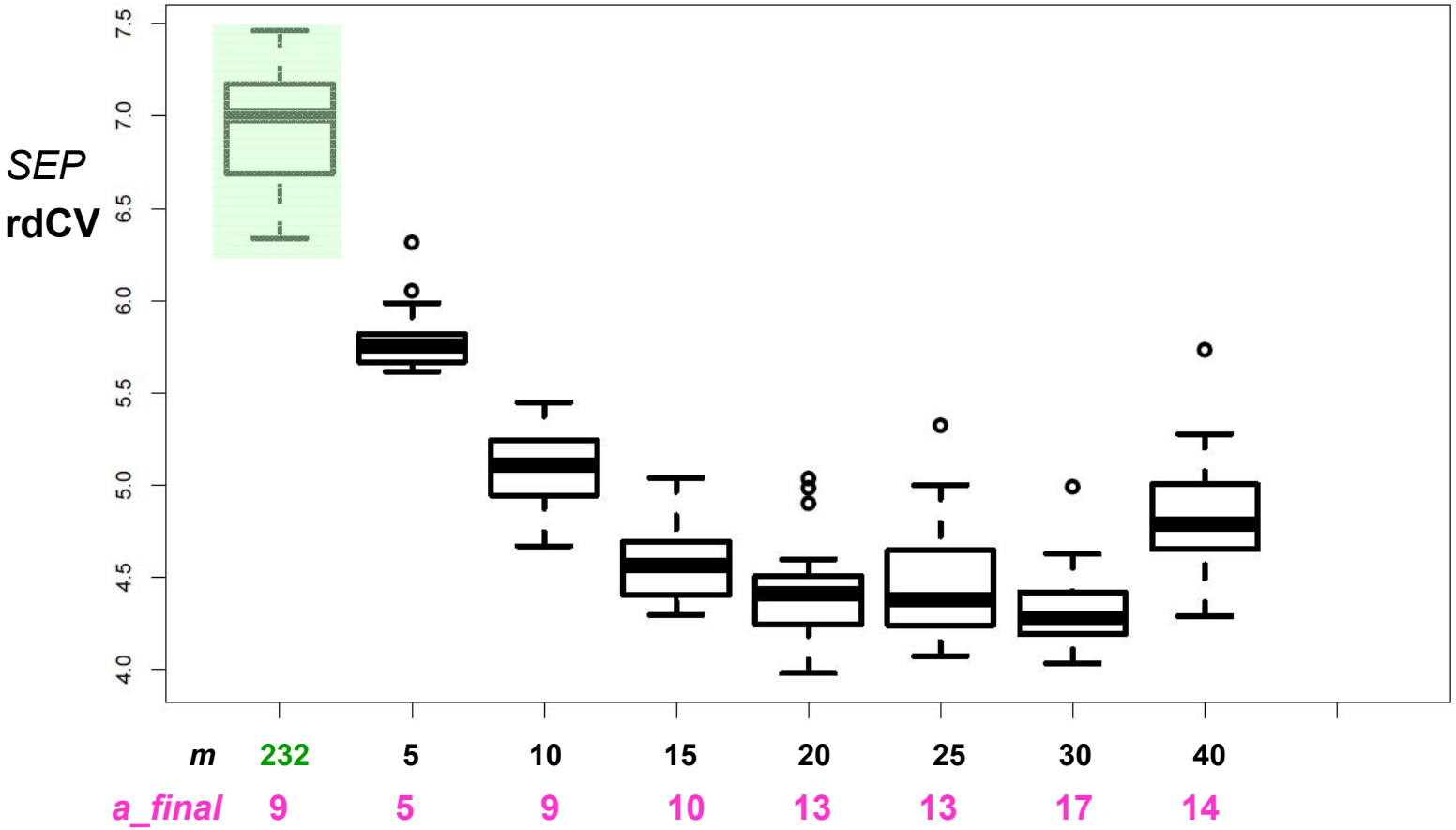


Cadima, J. et al.: Computational aspects of algorithms for variable selection in the context of principal components. *Computational Statistics & Data Analysis*, 47, 225-236 (2004).

Variable Selection: Genetic Algorithm (GA)

Criterion (fitness): $R^2(y, \hat{y})$, **Pearson (!)** **[R-library *subselect; genetic()*]**

Data: **GLU-NIR** (166 × 232)



VS: GA, gen=300, mutat.prob.=0.01; **rdCV:** rep=30, amax=20

Variable Selection: All subsets + rdCV

Criterion: SEP (rdCV)

Data: **HEAT-ELE** (122 × 13)

Variables		Best subsets (SEP_{FINAL} from rdCV)					
No.	Name	1 st	2 nd	3 rd	4 th	5 th	**20 th**
1	C						
2	H	■	■	■	■	■	■
3	N	■	■	■	■	■	
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5	C*H	■	■	■	■	■	■
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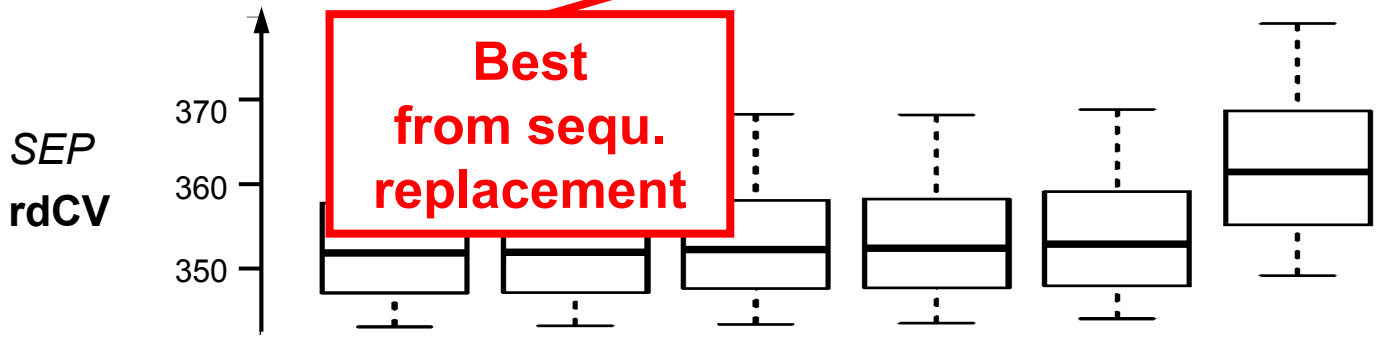
Best subset regression

Best from sequ. replacement

Best with GA



Variable Selection: Genetic Algorithm (GA)

Criterion (fitness): $R^2(y, \hat{y})$, Pearson (!) [R-library *subselect; genetic()*]

Significant improvement of prediction performance.

Very time consuming.

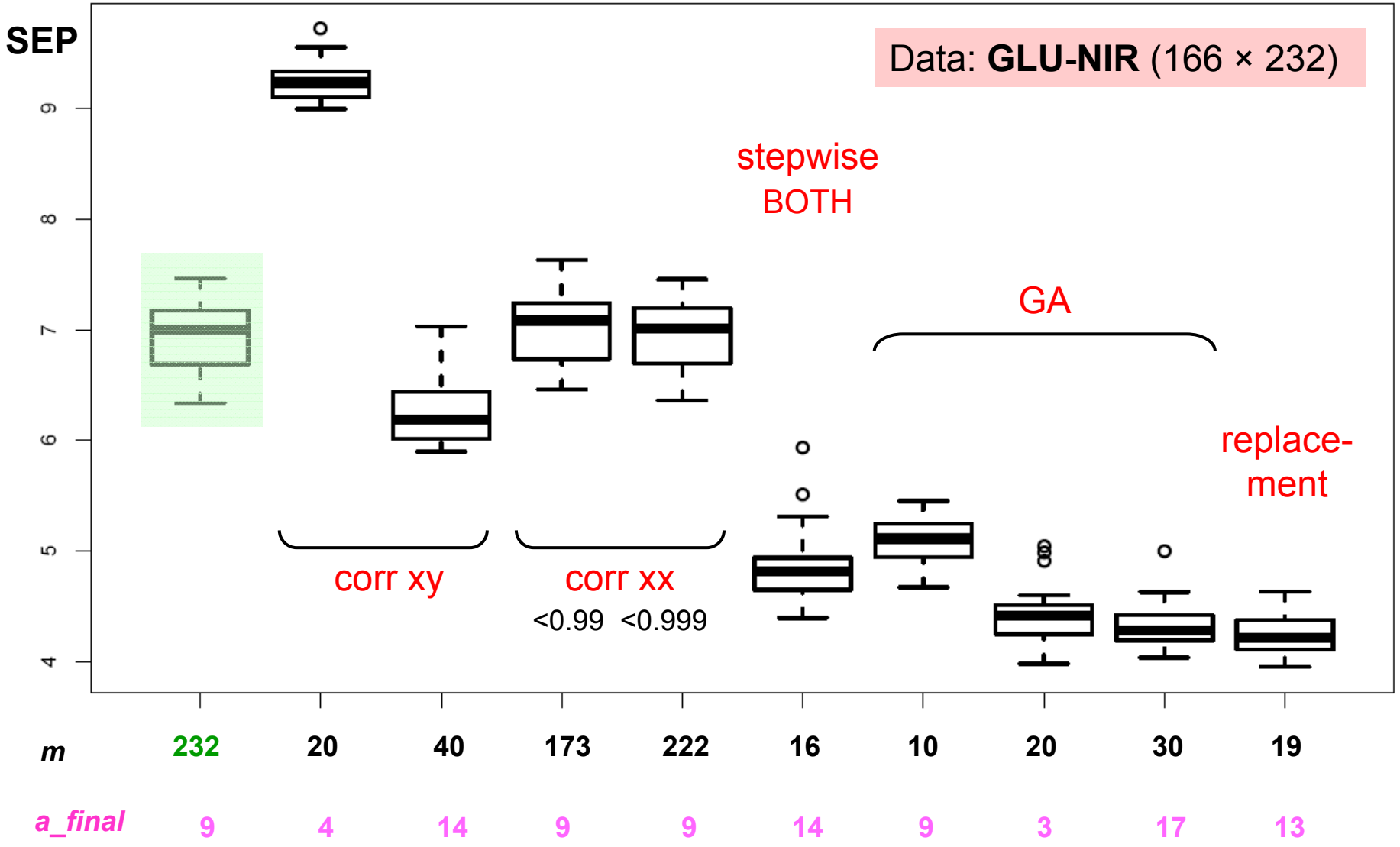
Rather not appropriate for m >500.

Variable Selection Methods

- all subsets
- best subset regression
- highest correlation with *y*
- highly correlating *x*-variables
- stepwise selection
- replacement
- genetic algorithm
- **many others**

- Monte Carlo (purely random),
- lasso regression, elastic net,
- VIP (variable importance in PLS),
- random forest,
- simulated annealing,
- particle swarm optimization,
- ant colony optimization,
- . . .
- ***tempting names (myth?) ...***

Selected best variable selection methods



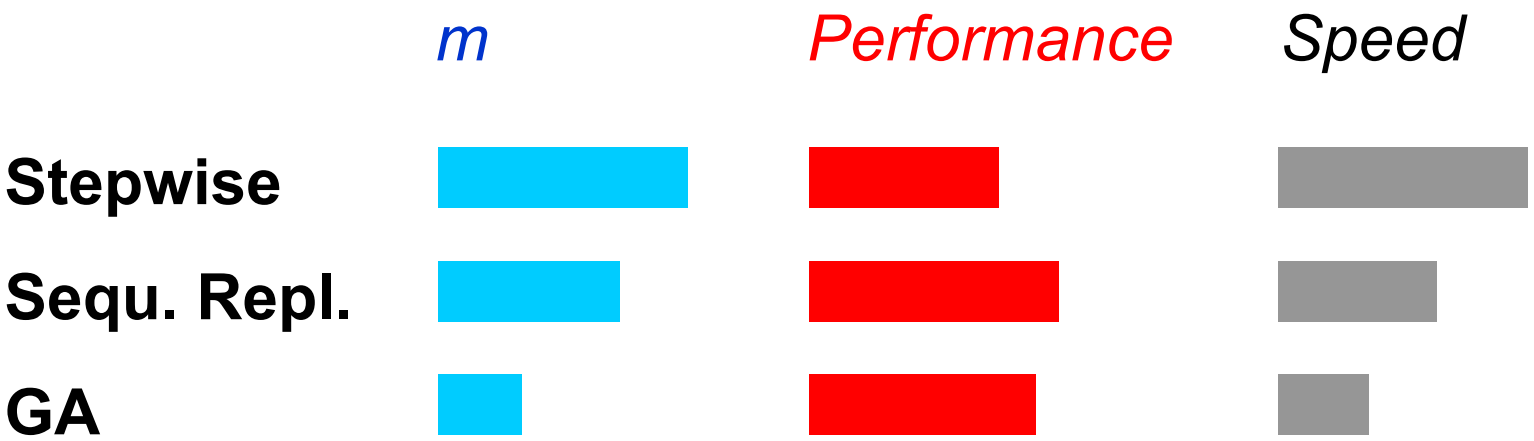
Conclusions

Variable selection often improves the model performance; however, mostly not dramatically.

Usually, no strategy is known for choosing an optimal variable selection method for a given data set.

- **Try several methods and vary parameter(s), resulting in several (many) variable subsets.**
- **Test these suggestions carefully in a similar way as the model will be applied (usually estimate the performance for test set objects - perhaps by rdCV).**

Promising methods for variable selection

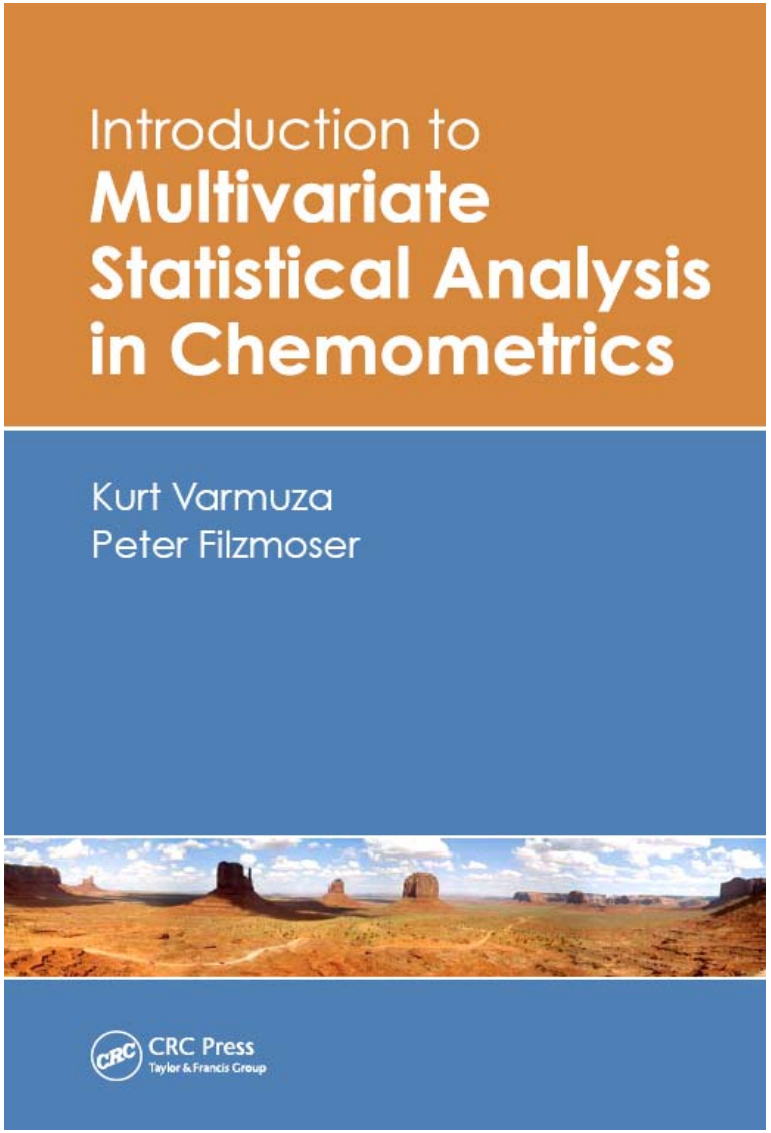


Conclusions may depend on used data sets.

Remember:

Usually, no guarantee for global optimal solution.

Thanks for collaboration: Peter Filzmoser (TU Vienna)



CRC Press, Taylor & Francis Group,
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Ca 320 pages,
appr. € 100

Includes many R-codes (examples, data)

Methods are explained without using R

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