Variable Selection

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Outline

- Why select variables?
- What methods are there?
- So which to choose?
- In practice
- Some examples

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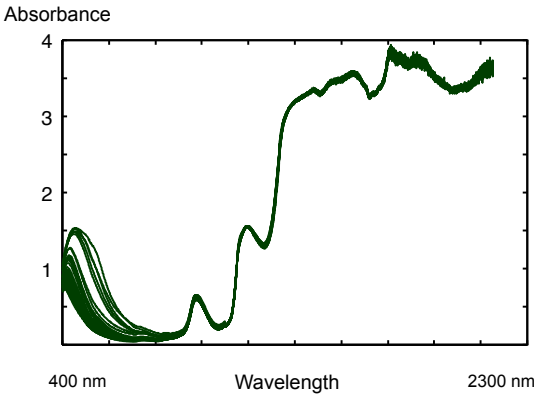
Why select
What methods
Choose method
In practice

VIS/NIR spectra of 61 beers

Purpose: prediction of real extract



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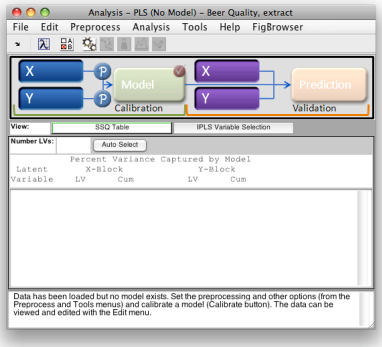
Why select
What methods
Choose method
In practice

VIS/NIR spectra of 61 beers

Try to make a PLS model for extract

- **Load beer.mat**
  - Calibrations X is in `beer` and Y in `extract`
  - Validation X is in `beertest` and Y in `extracttest`
  - Try to make a nice model and determine quality (RMSEC, RMSECV)



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Why select
What methods
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Exercise Data

Determination of the amount of extract from NIR spectra of beers.

Dispersive visual & near-infrared data collected (at 25 C) NIRSystems Inc. (Model 6500) spectrophotometer. Split detector system – silicon detector 400-1100 nm & (PbS) detector 1100-2500 nm.

VIS-NIR transmission recorded directly on undiluted degassed beer in 30 mm quartz cell. Spectral data collected at 2 nm intervals 400-2250 nm & converted to absorbance units.

Original *extract* concentration is a quality parameter in the brewing industry, indicating the substrate potential for the yeast to ferment alcohol and serving as a taxation parameter. Original extract concentration determined by Carlsberg A/S in the range of 4.23-18.76% plato.

Data sorted by extract value, and a model independent test set was constructed by selecting every third sample of this full data set. There are thus two data sets: one for calibration (40 samples) and one for independent estimation of prediction error (20 samples).

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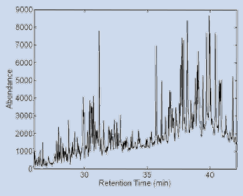
Why select
What methods
Choose method
In practice

Why variable selection?

- Improvement of the model
  - Remove irrelevant, unreliable or noisy variables
  - Improve predictions
  - Improve statistical properties
- Interpretation
  - Obtain a model that is easier to understand
- Costs
  - Use less measurements to replace expensive or time-consuming one
- Development of fast instruments/routines for on-line control
  - Find wavelength ranges for a filter-based instrument



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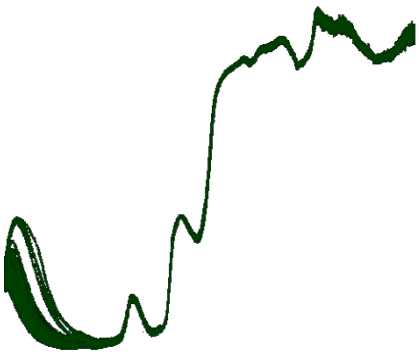
Why select
What methods
Choose method
In practice

What methods available?

- **A priori**
  - Choose measurements
- **A posteriori**
  - Use chemical/physical insight
- **Model based**
  - Look at loadings
- **"Random based"**
  - Genetic algorithms
  - Simulated annealing
- **Classical**
  - Forward, backward selection
  - Best subset selection
  - Significance tests
  - Significance based on Jack-knife
  - GOLPE
- **"Spectral"**
  - i-PLS
- **Other**
  - Pure variables
  - Principal variables
  - Iterative weighting with regression vector…



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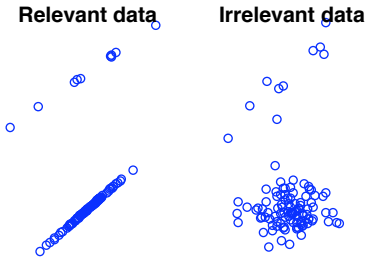
Why select
What methods
Choose method
In practice

What methods?

- Why not just choose the best variables?
  - Highly nonlinear problem
  - Exchaustive search not possible
  - How to validate what's good?

Best fitting variable of 1000 to ten calibration samples

New data (100 samples)



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Method : A priori

Choose the right measurements

- The most important of all
- Beyond the scope of this course as we assume the data are already available/fixed

Important assumptions

- There may be indirect correlations that you did not anticipate
- Don't choose too few variables a priori

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Method: A Priori

Example indirect relation

JOURNAL OF CHEMOMETRICS
J. Chemometrics 2002; 16: 451–463
Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/cem.735

Screening for dioxin contamination in fish oil by PARAFAC and N-PLSR analysis of fluorescence landscapes†

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Food Technology, Department of Dairy and Food Science, Royal Veterinary and Agricultural University, Rolighedsvej 30, DK-1958 Frederiksberg C, Denmark

Received 2 September 2001; Revised 28 February 2002; Accepted 4 April 2002

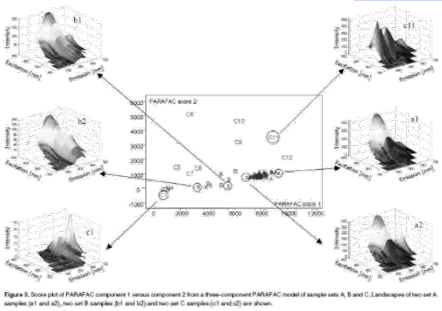

Figure 3. Score plot of PARAFAC component 1 versus component 2 from a three-component PARAFAC model of sample sets A, B and C. Landscapes of two set A samples (a1 and a2), two set B samples (b1 and b2) and two set C samples (c1 and c2) are shown.

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Method: A Priori

Why select
What methods
Choose method
In practice

Example indirect relations

Even though not direct link – fluorescence works well!!!

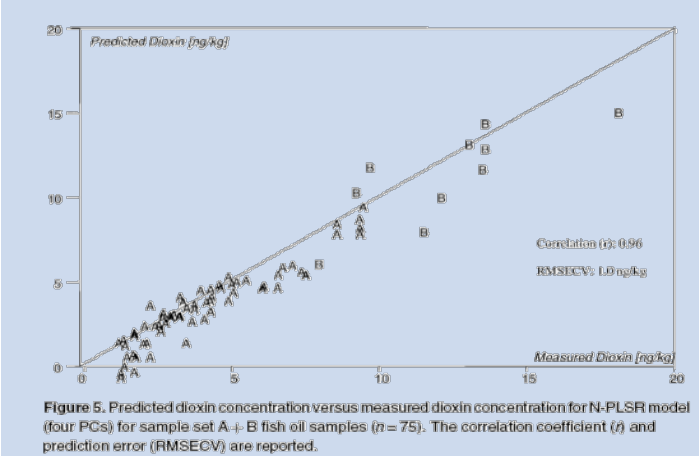

Figure 5. Predicted dioxin concentration versus measured dioxin concentration for N-PLSR model (four PCs) for sample set A + B fish oil samples ($n = 75$). The correlation coefficient (r) and prediction error (RMSECV) are reported.

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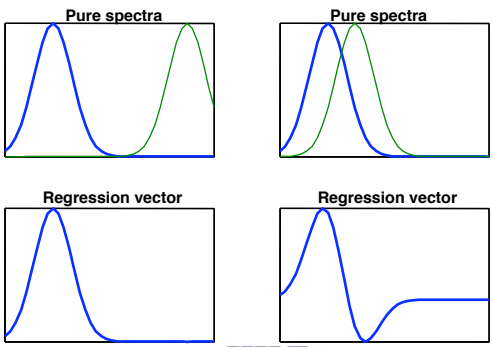
Why select
What methods
Choose method
In practice

Method : A posteriori

- Remember that a regression model is not only depending on the analyte directly
- Also has to adjust for overlapping signals



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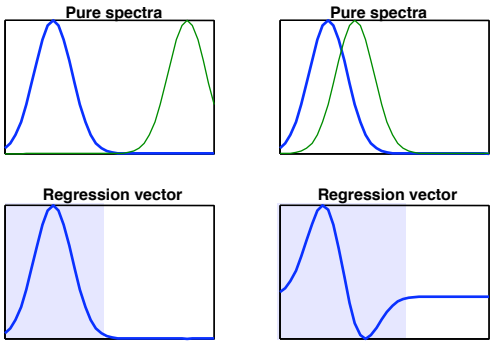
Method : A posteriori

- Remember that a regression model is not only depending on the analyte directly
- Also has to adjust for overlapping signals



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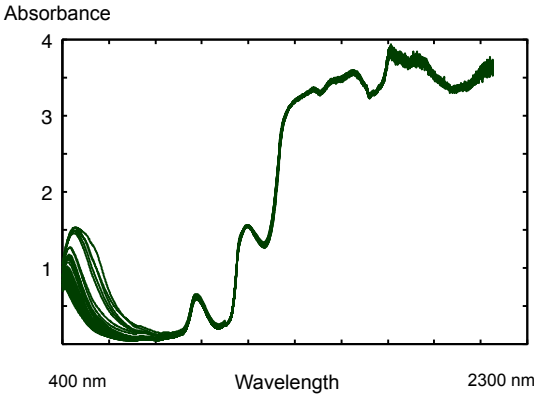
Example: A posteriori

VIS/NIR spectra of 61 beers

Purpose: prediction of real extract



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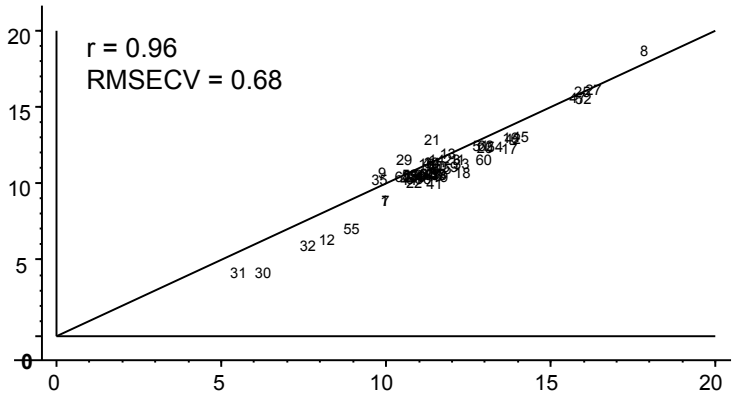
Example: A posteriori

Full spectrum PLS-model

Cross validated prediction error (61 samples, 6 segments)
Five PLS factors



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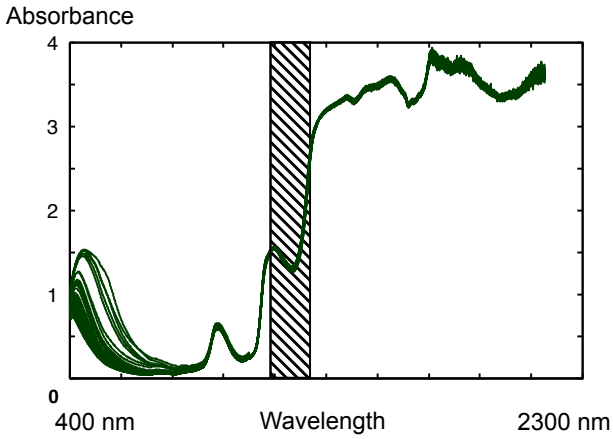
Example: A posteriori

Selected interval: 1218-1300 nm



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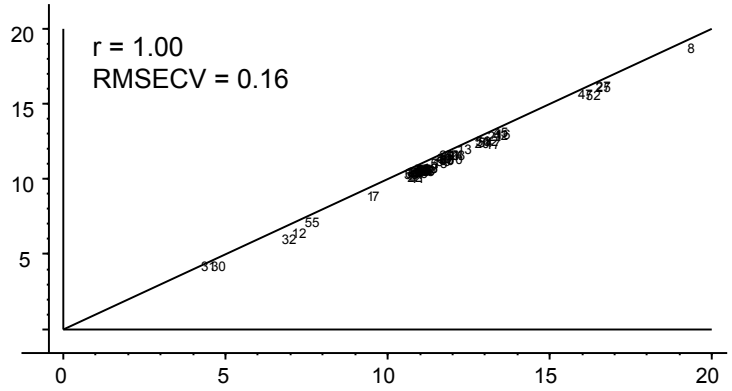
Example: A posteriori
PLS-model based on 1218-1300 nm

Cross validated prediction error (61 samples, 6 segments)
Three PLS factors



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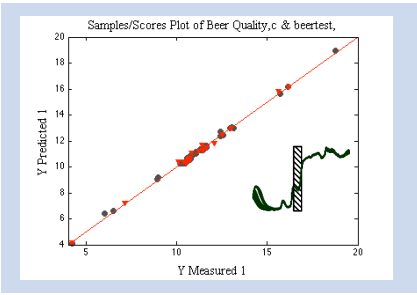
Why select
What methods
Choose method
In practice

Example: A posteriori
PLS-model based on 1218-1300 nm

This course is about how to achieve results as these even in situations where such detailed background knowledge is not accessible.



RMSEC = 0.13
RMSECV = 0.15
RMSEP = 0.17

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Model based selection

- Simply use the visual appearance of the model
- E.g. small loadings, low regression coefficents etc.

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Model based selection
Important assumptions

- **Model is reasonable**
  - if 900 out of 1000 variables irrelevant, the model may be reflecting those and hence the relevant ones look insignificant
- **Model is certain**
  - Few samples or noisy measurements =>
  - Statistical uncertainty high =>
  - Do not trust the model parameters too much

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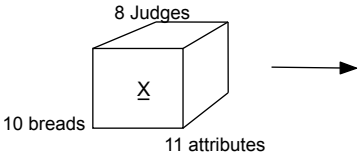
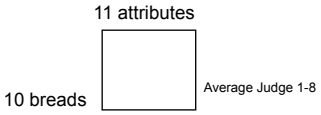
Model based selection
Example – Sensory analysis

- Sensory profiling of bread
  - 10 breads (replicates) × 11 attributes × 8 judges
  - Average over judges: 10 × 11 attributes
  - Data from Magni Martens





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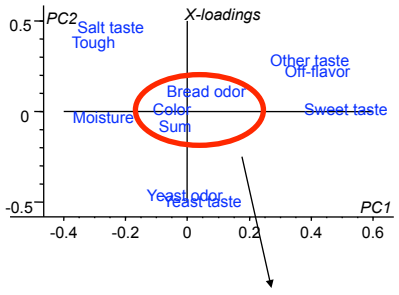
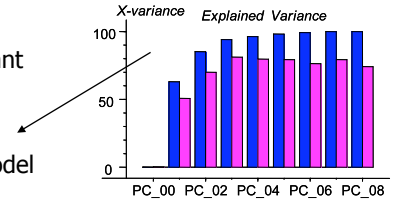
Model based selection
Example



Loadings indicate some variables not important



Seems trustworthy as the model is otherwise well-behaved

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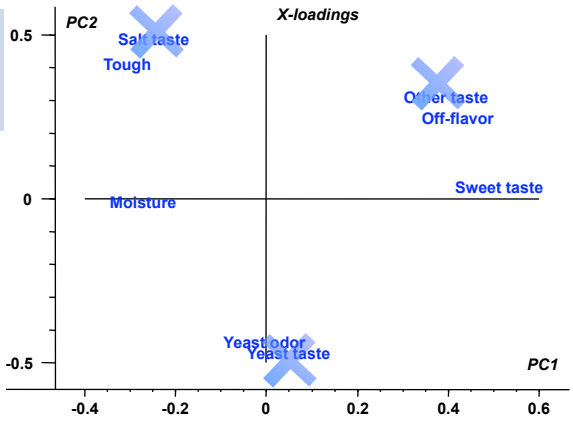
Model based selection
Example - Many ways to skin a cat

Want to get rid of more?

Remove redundant variables



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Model based selection
Automating it a bit

Variable importance for projection (VIP)

Relative weighted sum of squares of PLS-weights, weighted by components importance for predicting

- Assumes valid model
- Hence only remove few variables at a time
- And check for outliers etc. along the way
- VIP smaller than one indicates low importance

S. Wold, E. Johansson, M. Cocchi, 3D QSAR in Drug Design; Theory, Methods, and Applications, ESCOM, Leiden, Holland, 1993, pp. 523– 550.

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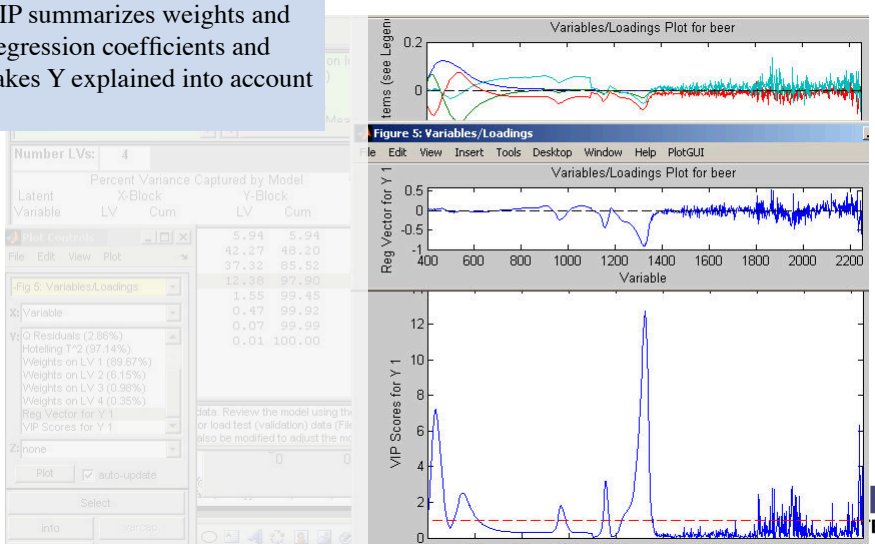
Why select
What methods
Choose method
In practice

Model based selection
Automating it a bit

VIP summarizes weights and regression coefficients and takes Y explained into account



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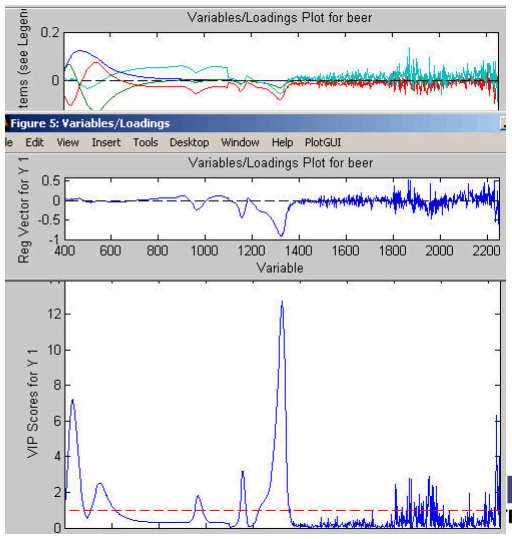
Model based selection
Automating it a bit

Why select
What methods
Choose method
In practice

Try yourself on the beer data.

Is a one-shot selection optimal?



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"Random" variable selection

Random selection means choosing without considering improvement in fit directly

Increases chance of obtaining unforeseen and complex interactions

Genetic algorithms is a good example

home > in the lab > article

Genetics Help Breed Best Missile Designs

By Jim Bowne

Huntsville, Ala.-The Army Aviation and Missile Research, Development and Engineering Center is concerned about shrinking research and development funds. The center also is concerned about receiving increased requirements to design, analyze and develop complex missile systems that have shortened timelines. However, the center continues to develop creative solutions.

The Compact Kinetic Energy Missile is among the missiles that benefit from the use of genetic algorithms, which automate and streamline the missile design process.

www.rdecom.army.mil

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Genetic algorithm

- **Method**
  - Survival of the fittest (best fit)
- **Principle**
  - Every combination of variables (a model) is defined by an index of which variables to use *and* the goodness of this model
    - *Example: One species is given by the calibration model with variable 1, 3, 14 & 27 yields and RMSEP of 1.23.*
  - Find better models by "mating" species so that the good ones mate more than bad ones (survival of the fittest).
    - *Example: Calibration models with variable 8 are generally better and therefore increasingly part of new calibration models.*

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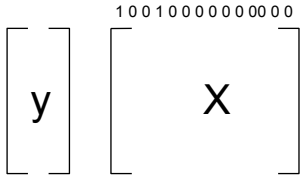
Genetic algorithm

- **Terminlogy**
  - Population = Set of individuals
  - One individual = Model with a given set of variables
  - One gene = Codes for one variable (in/out)

- **Algorithm**
  - Make start population (e.g. 50 different models with different variables included)
  - Evaluate each model (RMSEP or similar)
  - Have a party and let the best ones have most fun
  - Fun: two models mate and make a child which has similar variables
  - Arrange a new party for the 50 children and continue



Gene for one model defines which variables are in. RMSEP defines the quality of the individual

Riccardo Leardi has written many papers on how to make genetic algorithms work

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Random methods

Assumptions

- ”Random” methods are based on combining a random search (individuals) with a guided search (mating)
  - Mostly used because exhaustive search is too expensive
  - Good and sound principle
  - Excellent for getting ideas
  - Not good, though, for refining

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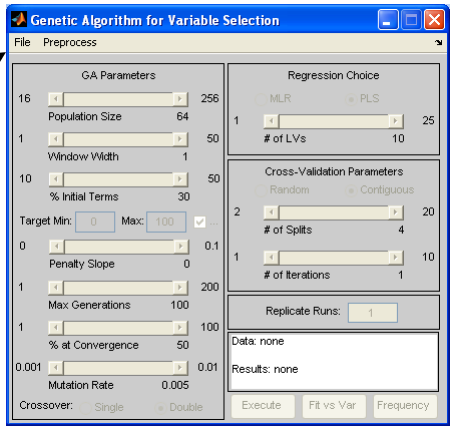
Genetic algorithms
Exercise

```
In MATLAB
>> load beer
>> genalg
```



- Load calibration data (beer and extract)
- Execute

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Why select
What methods
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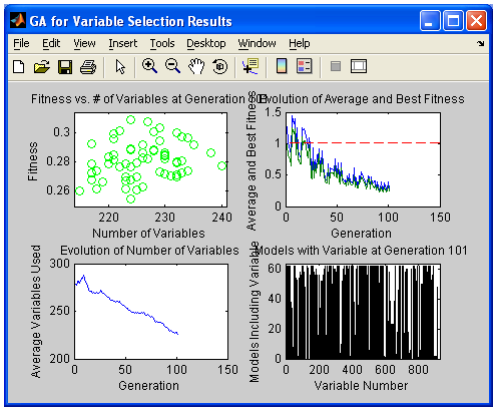
In practice

Genetic algorithms
Exercise

- Does the result look nice?
- Maybe try increasing iterations?



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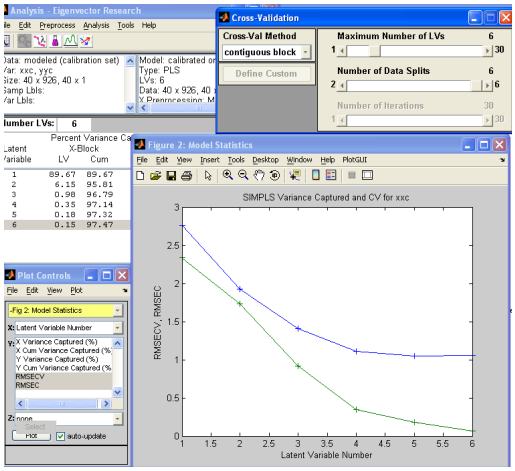
Genetic algorithms
Exercise

- **Generally**
- Lower the number of components based on initial PLS analyses but use a little more
- Keep ending criteria sensitive. The more iterations which occur, the more feedback from the cross-validation information, thus more likely over-fitting,
- Use random cross-validation and multiple iterations if practical,
- Repeat the GA run multiple times and watch for general trends
- For data with many variables and fewer samples, increase the window width



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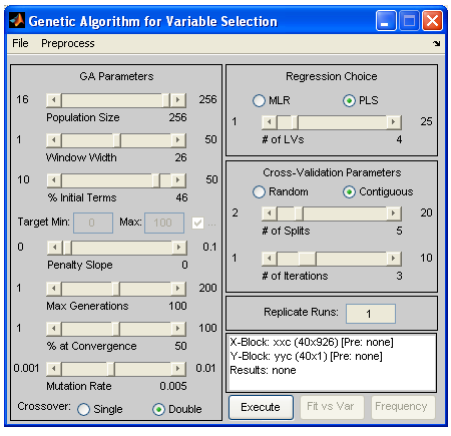
Genetic algorithms
Exercise

- **In PLSToolbox**
- **Size of Population** Larger populations provide a better representation of different variable combinations.
- **Window Width** When adjacent variables contain correlated information the original variables can be included or excluded in "blocks".
- **% Initial Terms** Appr. # variables included in the initial subsets. Few initial terms will make identification of useful variables more difficult, but will bias the end solution towards models with fewer variables.
- • **Target Min/Max & Penalty slope** For guiding towards a specific number of variables



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Why select
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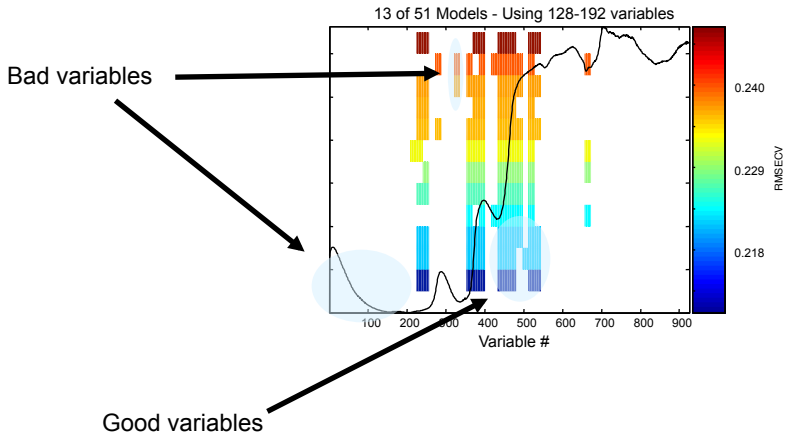
Genetic algorithms
Exercise



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Why select
What methods
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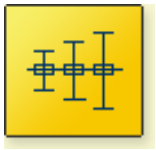
In practice

Classical methods

- Subset selection
  - Statistical significance tests
  - Forward selection
  - Backward selection
  - Best subset selection



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Classical methods

Statistical significance tests

Principle

- Do regression
- Eliminate variables with non-significant regression coefficients

Properties

- Very fast
- Assumes a statistically valid model
- Assumes statistically valid significance tests
- Hence only works for models with insignificant amount of irrelevant variables

The function `Calibsel` selects variables based on significance

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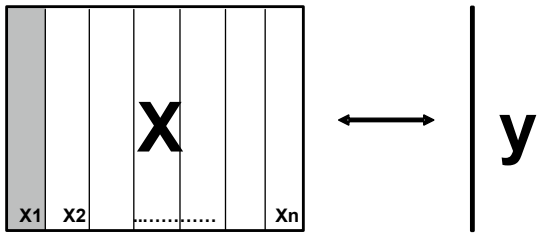
Intermezzo

iPLS: Interval PLS

Local models in n intervals. Very intuitive and useful approach that can be easily combined with variable selection



L. Nørgaard, A. Saudland, J. Wagner, J. P. Nielsen, L. Munck, S. B. Engelsen. Interval partial least-squares regression (iPLS). *Appl.Spectrosc*. 54 (3):413-419, 2000.

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Why select
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Classical methods
Forward selection

- **Principle**
  - Select best fitting variable (or better cross-validated)
  - Regress y on this and select variable fitting best on residual
  - Regress y on these two and select best fitting on the residual
  - Etc.
- **Good**
  - Fast
  - Handles many irrelevant variables
    - If many samples or test set evaluation
  - Works well sometimes!
- **Bad**
  - Disregards interactions to some extent

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Why select
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In practice

Forward selection
Exercise

- **Try forward selection on NIR data**

- **Many variables – computationally expensive**
  - If correlation between neighbors use windows instead of individual variables.
  - E.g. use every 10 neighbors as one set and ex/include them all together

Use the algorithm `IPLS` to do variable selection

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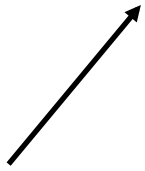
Forward selection
Exercise


```
In MATLAB
>> load beer
>> help ipls
>> width = 20;
>> lv = 4;
>> [use,fit,lvs,int] = ipls(beer,extract,width,lv);
```



Divide into intervals of 20 variables width

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Forward selection
Exercise


```
In MATLAB
>> load beer
>> help ipls
>> width = 20;
>> lv = 4;
>> [use,fit,lvs,int] = ipls(beer,extract,width,lv);
```

Maybe more than one interval could be useful.

Use the options in ipls to select more than one interval.

Divide into intervals of 10 variables width

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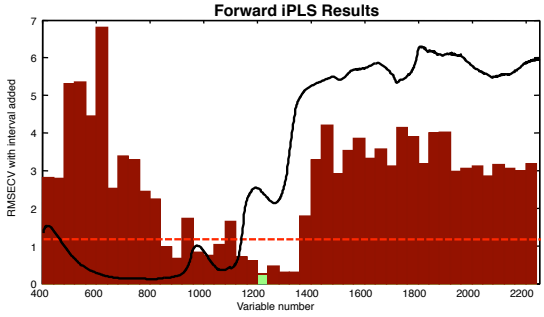
Forward selection
Exercise

```
In MATLAB
>> myopt = ipls('options');
>> myopt.numintervals  = 3;
>> myopt.preprocessing  = 'meancenter';
>> [use,fit,lvs,intervals] = …
      ipls(beer,extract,width,lv,myopt);
```



Forward selection
Exercise

Number of intervals
Should it perhaps be 2 or 8?
Let ipls check it

```
In MATLAB
>> myopt.numintervals  = Inf;
>> [use,fit,lvs,intervals] = …
      ipls(beer,extract,width,lv,myopt);
```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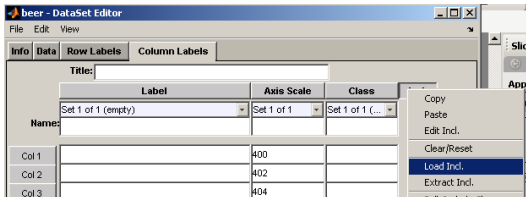
Forward selection
Exercise

Use the solution and check in PLS

Open `beer` in data set editor and load `use` as new include field for variables and save e.g. as `beer2`. Do a PLS model and see if predictions are fair

```
>> [use,fit,lvs,interval
   ipls(beer,extract,
```



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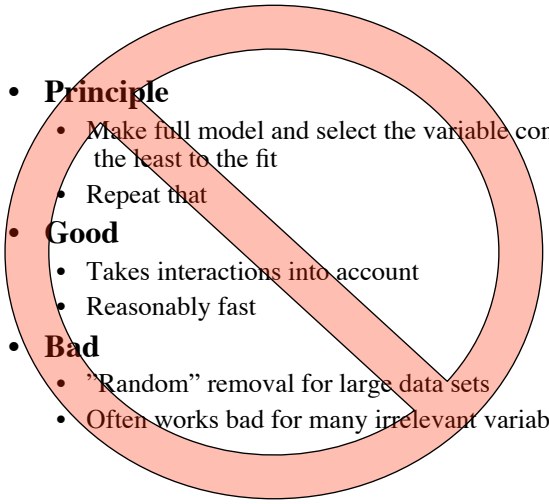
Classical methods
Backward selection



- **Principle**
  - Make full model and select the variable contributing the least to the fit
  - Repeat that
- **Good**
  - Takes interactions into account
  - Reasonably fast
- **Bad**
  - "Random" removal for large data sets
  - Often works bad for many irrelevant variables

Forward selection is usually better

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Choosing method

If there are many irrelevant variables

- Do not use tests based on statistics of overall model
  - Jack-knife, significance test, etc.
- The fewer samples, the more important the independence of the optimization criterion is
  - Do not use fit values but rather cross-validation or test set
- Genetic algorithms or forward selection are good choices
- Refine solution using background knowledge and other variable selection tools

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Choosing method

If refining an already ok model

- The more samples (to variables), the less important optimization criterion is
- Statistics makes sense
  - Significance is very helpful, model parameters can be interpreted meaningfully
- Use jack-knife, I-PLS, etc.

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Choosing method

If you have continuous or smooth data

Why select
What methods
Choose method
In practice

- Do not select individual variables but rather windows of variables
- Use I-PLS, genetic algorithms with window selection etc.

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Why select
What methods
Choose method
In practice

How to do it in practice

By now it is clear that most methods do not like outliers:

Remove outliers!!

Even if they are not finally removed, meaningful variable selection is not possible with even slightly significant outliers (unless very many samples).

So get rid of them and add them again afterwards

Alternative – robust methods

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How to do it in practice

- **Never trust results**
  - Use several methods as inspiration
  - Evaluate selected variables
    - Add some, remove some, check with a priori knowledge
- **The better the initial model, the better results from variable selection**
  - Remove obviously irrelevant variables
  - Remove outliers
  - Bin similar variables

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