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INTELLIGENT TECHNOLOGIES

Sensory profile of a salad dressing

Modelling by x**tractis**® fuzzy models

Sensometrics 2006 Workshop I

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xtractis® approach

- **Fuzzy** models
  - Modelling with few reference data (possibility theory)
  - May use incomplete databases (holes)
  - Interpretable models (compilation of linguistic rules)
  - Universal approximator of non linear function
- **Dimensionality** reduction
  - Only original variables of the process (no PCA)
  - Automatic reduction without any *a priori* knowledge
  - Allows model inversion (exact optimal input values)
- **Extensive use of robustness** estimation methods
  - Validation samples
  - Cross validation techniques
  - Selection of the most simple models

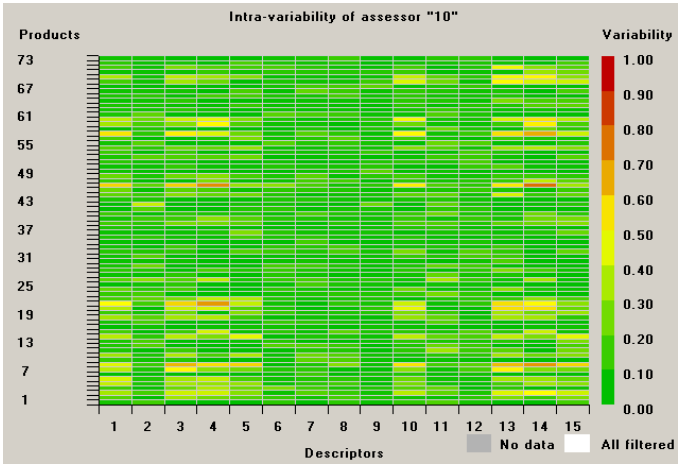
Input database formatting

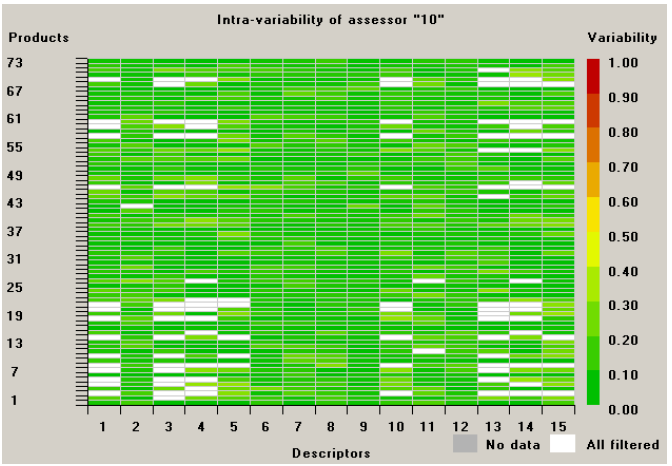
- Evaluation date translated into number of days
- Temperature condition replaced by temperature value
- Packaging material divided into 6 binary variables
  - Attributes are not numerical and not ordered
  - Database sample:

Evaluation date	Glass	PET	PP	Greaseproff paper	Aluinium foil	EVOH	Light	Temperature
135	0	0	0	1	0	0	0	23
197	0	0	0	1	0	0	0	23
244	0	0	0	1	0	0	0	23
307	0	0	0	1	0	0	0	23
0	0	0	0	0	1	0	0	23
62	0	0	0	0	1	0	0	23
135	0	0	0	0	1	0	0	23
197	0	0	0	0	1	0	0	23
244	0	0	0	0	1	0	0	23
307	0	0	0	0	1	0	0	23
0	0	0	0	0	0	1	0	23
62	0	0	0	0	0	1	0	23
135	0	0	0	0	0	1	0	23
197	0	0	0	0	0	1	0	23
244	0	0	0	0	0	1	0	23

Output database filtering (1/2)

- **Intra-variability** analysis (between repetitions of the same evaluation)

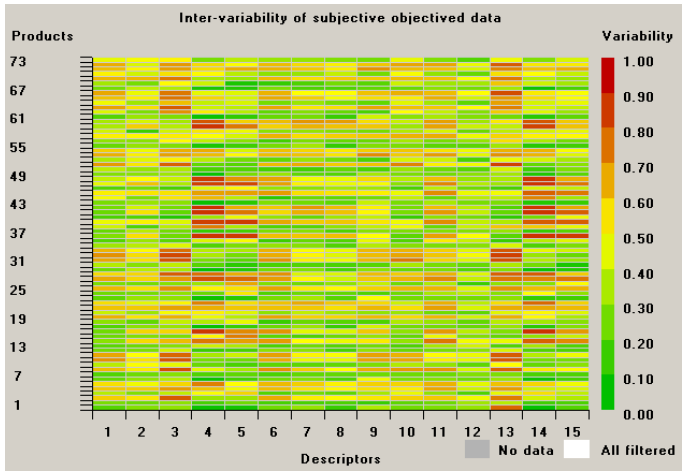


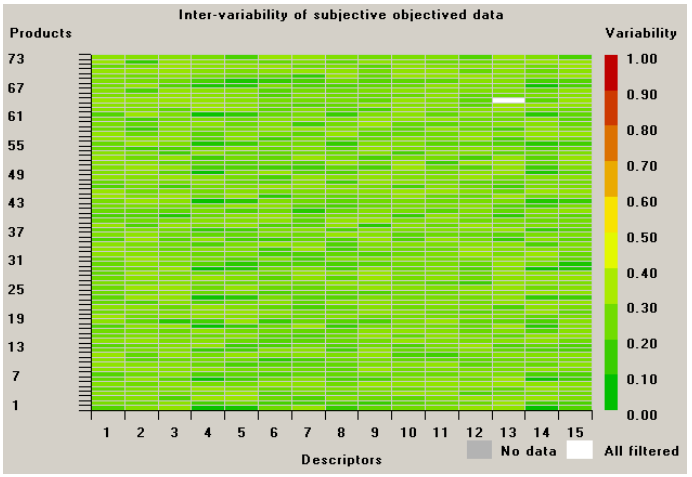


- Filtering of repetitions
  - If 2 repetitions of the same evaluation differ by more than X% of the definition range, they are discarded
    (X=35%, 3.2% of scores discarded)
  - Aggregation of repetitions to get the best estimation of the assessor's evaluation

Output database filtering (2/2)

- **Inter-variability** analysis (between experts for the same descriptor)





- Filtering of assessor's evaluations
  - Algorithm to select the biggest cluster of scores with a variability lower than X% of the definition range
    (X=40%, 2.5% of scores discarded)
  - Aggregation of experts' evaluations to get the best estimation of descriptor value

Structure of a fuzzy model (1/3)

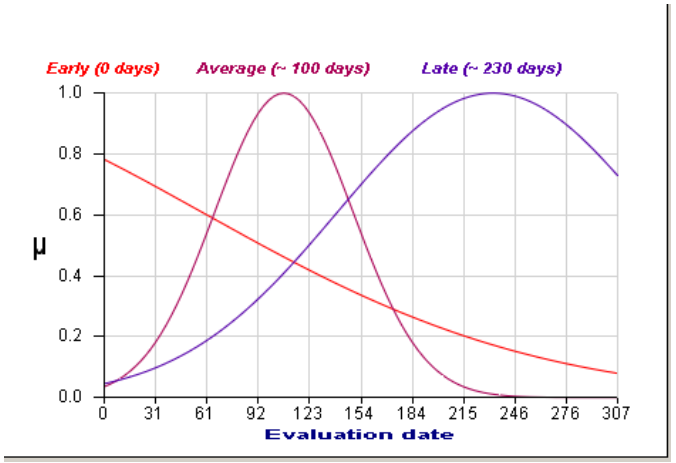
- **Input** variables
  - Only original variables (no principal components)
  - Variable selection in relation with the process output
- **Rule** base
  - Inference made according to linguistic rules
  - *Example*: a fuzzy rule used to predict descriptor *Sour odour*

If	Evaluation date	is	*Late*					
And	Packaging	Is	0.5	0.5	1	0.3	0.5	0.5
			Glass	PET	PP	GPP	Al	EVOH
And	Light	is	*False*					
Then	Sour Odour	is	*Low*					

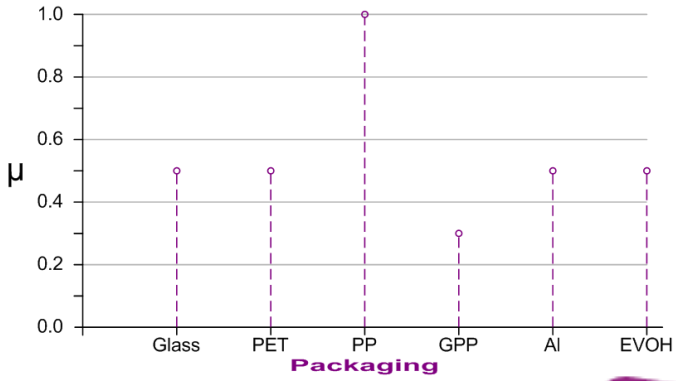
  - Premises of rules = fuzzy sets

Structure of a fuzzy model (2/3)

- **Input** partitions
  - Each variable qualified by fuzzy classes
  - *Example*: variable *Date*
  - Fuzzy partition of a continuous set



  - *Example*: variable *Packaging*
  - Fuzzy partition of a discrete set



Structure of a fuzzy model (3/3)

- **Rule** conclusions
  - Scalar (crisp) values
  - *Example*: descriptor *Sour odour*

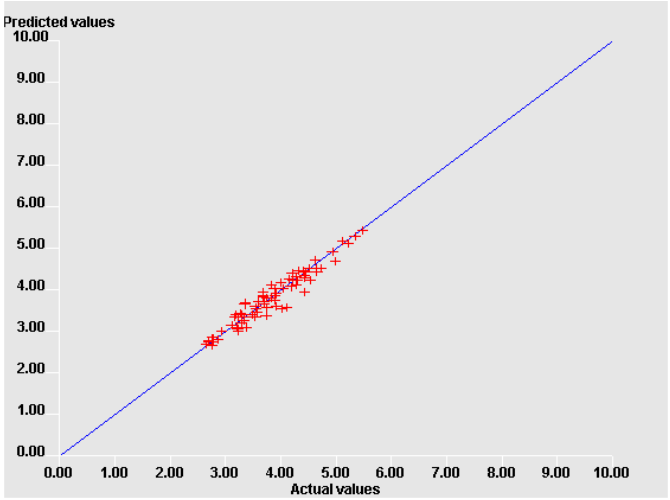
Name	Type	Value
Very low	*const*	3,39
Low	*const*	3,58
High	*const*	6,33

Model performance evaluation (1/5)

Accuracy

- Ability to predict learning samples
- Easy to achieve
- *Example*: *Color intensity*

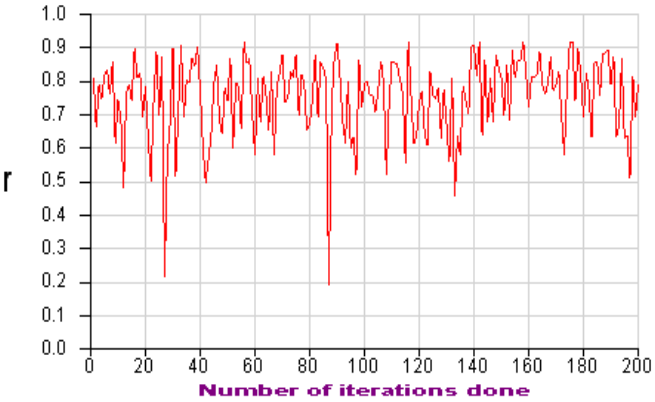
Correlation coefficient	0,965
Mean error (predicted - actual)	-0,02
Error standard deviation	0,179
Hamming's error	1,37 %
Maximum error	5,16 %
Mean mapping degree (data)	0,384
Min mapping degree (data)	0,163
Non mapped data count	0 (0 %)



➡ Insufficient performance index because of overfitting phenomenon

Model performance evaluation (2/5)

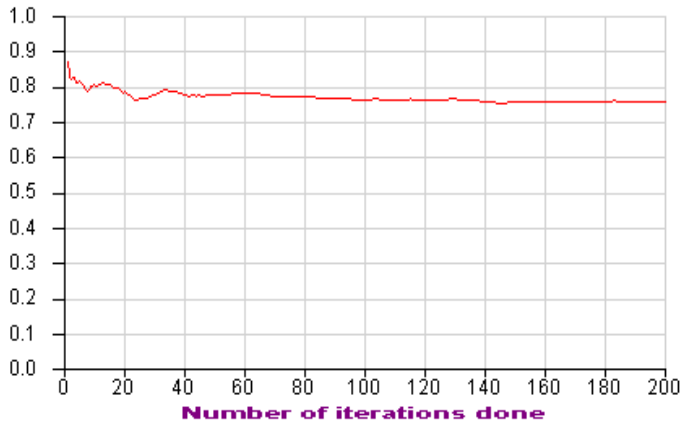
- **Robustness** analysis
  - Necessary to detect overfitting phenomenon
  - Several methods to estimate the generalization capacity
- **Validation sample** (most widely used)
  - Several drawbacks of "2/3 - 1/3 split":
    - 1/3 data not used for learning
    - Strong sensitivity to choice of the validation sample
  - *Example*: robustness of the same learning structure applied on 200 randomly selected learning sets (leave 30% validation points out)



Model performance evaluation (3/5)

Cross validation

- Whole database used for the model generation
- Same learning structure (model structure, learning parameters) applied on a large number of learning/validation splits
- Robustness estimation computed on the scatter of validation points of all models (convergence ~ 50 to 300 iterations)
- Computationally intensive, but insensitive to an arbitrary choice of learning and validation base
- x**tractis**® preferably uses cross validation techniques
- *Example*: Robustness of learning structure



Model performance evaluation (4/5)

Compactness

- With similar accuracy and robustness, always select the simplest model
- Increases interpretability
- Reduces risk of overfitting

- *Example*: 2-rules model to predict *Off-odour*

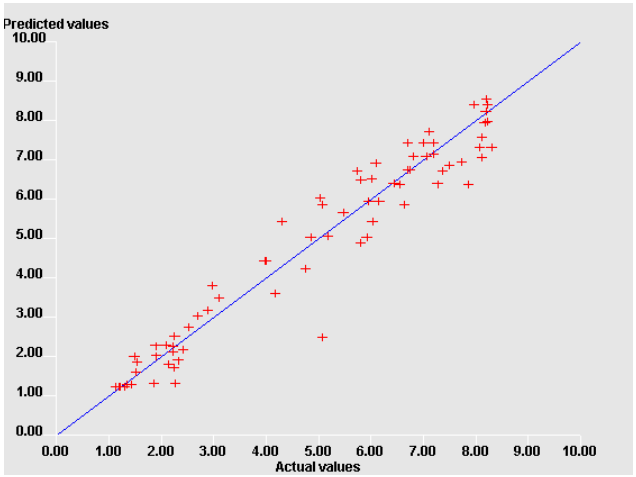
If	Evaluation date	is	*Late*					
And	Packaging	Is	0.7	0.7	1	0.7	0.3	0.7
			Glass	PET	PP	GPP	Al	EVOH
And	Light	is	*True*					
And	Temperature	is	*High*					
Then	Off- Odour	Is	*High*					

If	Evaluation date	is	*Early*					
And	Packaging	Is	1	1	0.55	1	1	1
			Glass	PET	PP	GPP	Al	EVOH
And	Light	is	*false*					
Then	Off- Odour	Is	*low*					

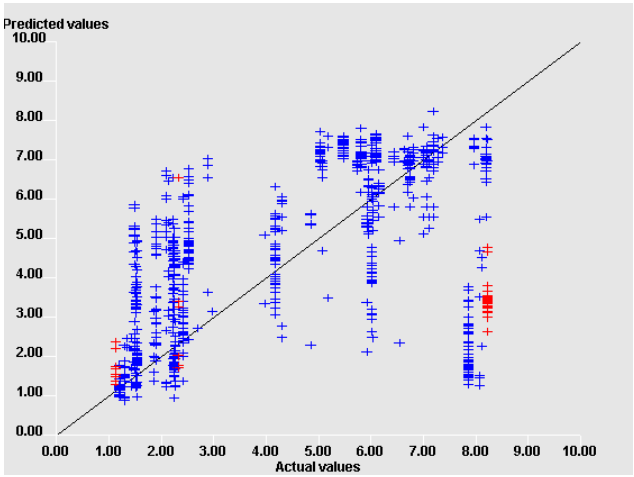
Model performance evaluation (5/5)

Importance of robustness evaluation

- Really easy to get an accurate model with a very poor robustness
- The model is specific to the available learning points: it does not actually model the process
- *Example*: accurate & non robust model for *Fresh flavour*



r=0.968



r=0.517

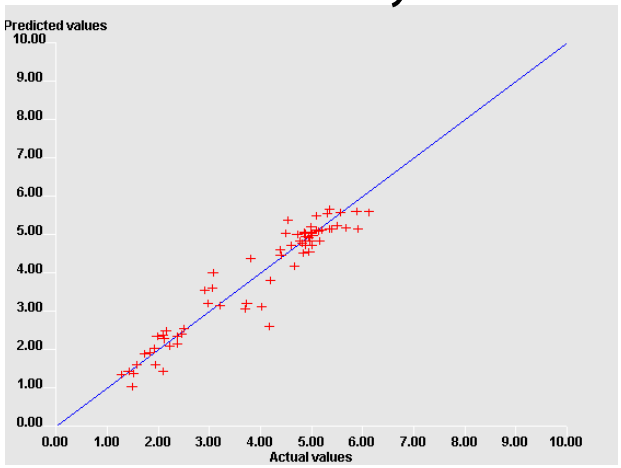
Overview of the results

- 6 sensory attributes (out of 15) are difficult to model
  - *Sour odour*, *Rancid odour*, *Off odour*, *Sour flavour*, *Fresh flavour, Sweetness*
  - Difficult to reach a good robustness
  - Most robust models not very accurate

Best models for whole sensory profile

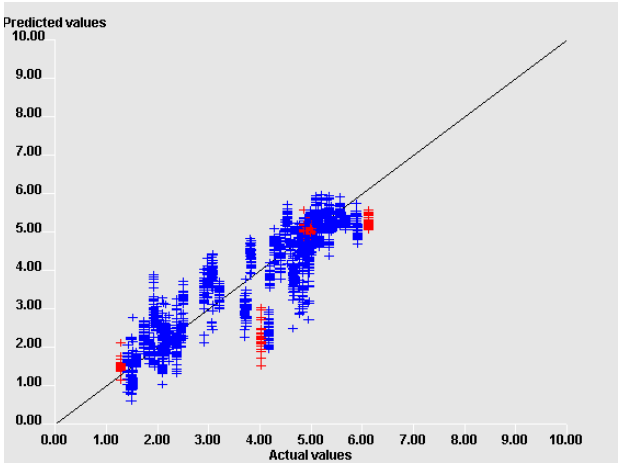
Acidic odour ☺

Accuracy



Correlation coefficient	0,960
Mean error (predicted - actual)	-0,03
Error standard deviation	0,404
Hamming's error	2,90 %
Maximum error	15,63 %
Mean mapping degree (data)	0,513
Min mapping degree (data)	0,198
Non mapped data count	6 (8 %)

Monte Carlo 20%-CV

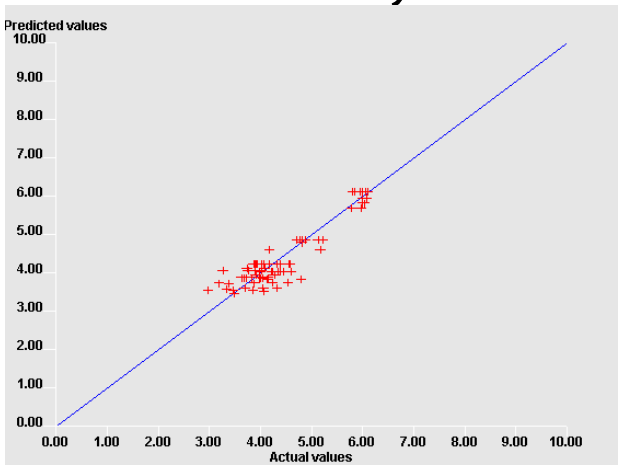


Correlation coefficient	0,905
Mean error (predicted - actual)	-0,06
Error standard deviation	0,606
Hamming's error	4,48 %
Maximum error	24,97 %
Mean mapping degree (data)	0,428
Min mapping degree (data)	0,101
Non mapped data count	52 (2 %)

Best models for whole sensory profile

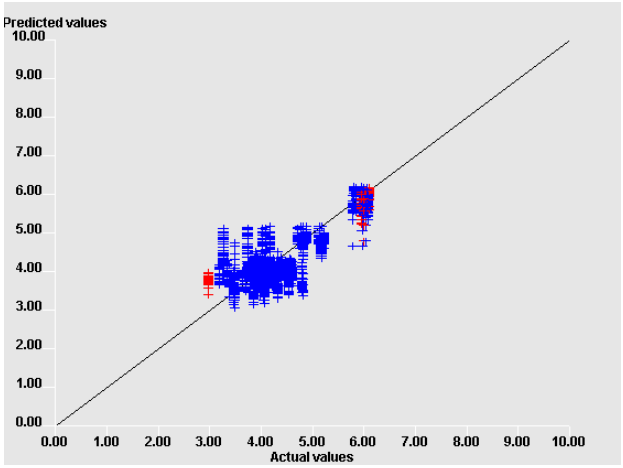
Sour odour ☹

Accuracy



Correlation coefficient	0,915
Mean error (predicted - actual)	-0,04
Error standard deviation	0,332
Hamming's error	2,63 %
Maximum error	9,69 %
Mean mapping degree (data)	0,567
Min mapping degree (data)	0,190
Non mapped data count	1 (1 %)

Monte Carlo 20%-CV

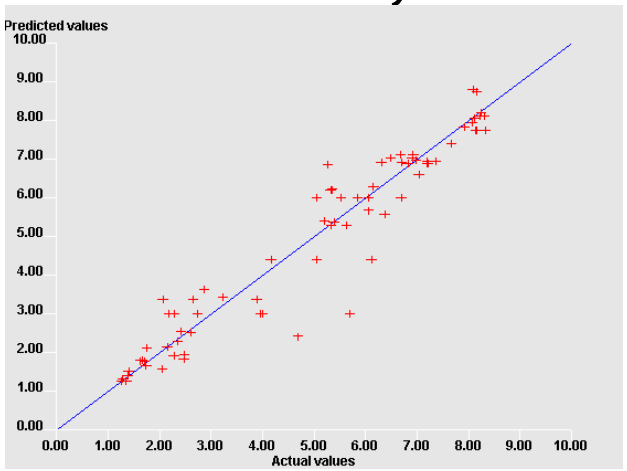


Correlation coefficient	0,840
Mean error (predicted - actual)	-0,05
Error standard deviation	0,452
Hamming's error	3,53 %
Maximum error	18,70 %
Mean mapping degree (data)	0,532
Min mapping degree (data)	0,108
Non mapped data count	20 (1 %)

Best models for whole sensory profile

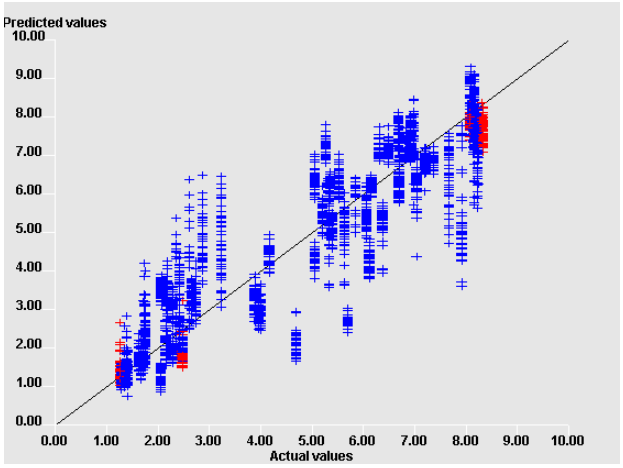
Fresh odour ☺

Accuracy



Correlation coefficient	0,960
Mean error (predicted - actual)	-0,04
Error standard deviation	0,672
Hamming's error	4,49 %
Maximum error	26,89 %
Mean mapping degree (data)	0,557
Min mapping degree (data)	0,209
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

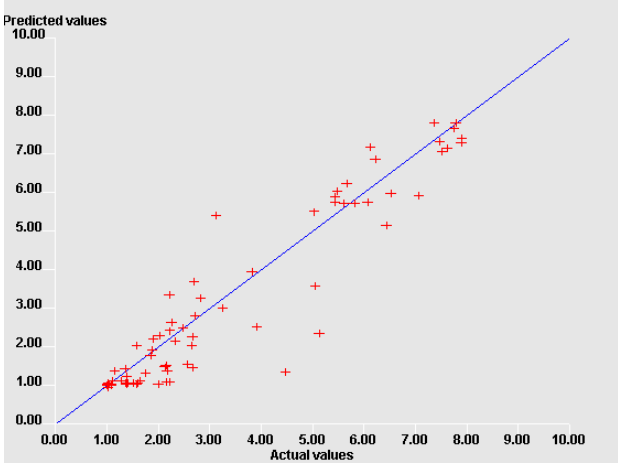


Correlation coefficient	0,907
Mean error (predicted - actual)	-0,04
Error standard deviation	1,008
Hamming's error	7,37 %
Maximum error	43,13 %
Mean mapping degree (data)	0,511
Min mapping degree (data)	0,101
Non mapped data count	81 (3 %)

Best models for whole sensory profile

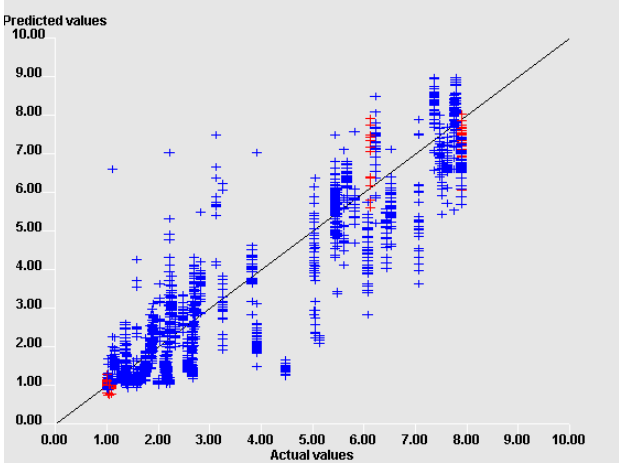
Rancid odour ☹

Accuracy



Correlation coefficient	0,944
Mean error (predicted - actual)	-0,20
Error standard deviation	0,774
Hamming's error	5,29 %
Maximum error	31,18 %
Mean mapping degree (data)	0,404
Min mapping degree (data)	0,152
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

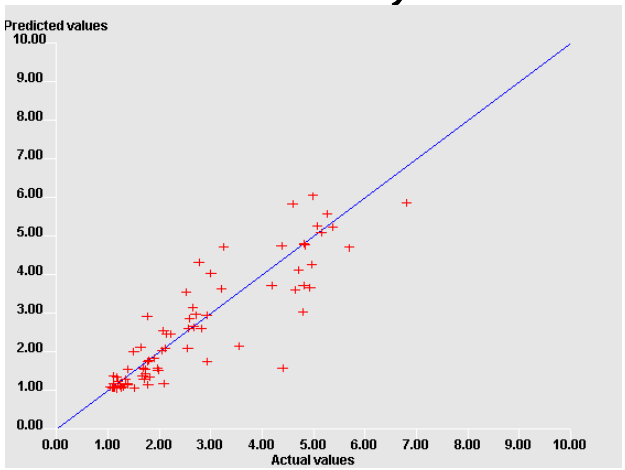


Correlation coefficient	0,927
Mean error (predicted - actual)	-0,17
Error standard deviation	0,880
Hamming's error	6,43 %
Maximum error	55,07 %
Mean mapping degree (data)	0,429
Min mapping degree (data)	0,101
Non mapped data count	307 (14 %)

Best models for whole sensory profile

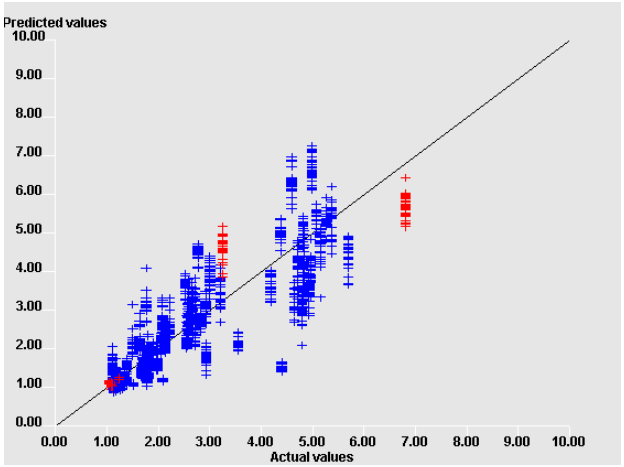
Off odour ☹

Accuracy



Correlation coefficient	0,889
Mean error (predicted - actual)	-0,09
Error standard deviation	0,701
Hamming's error	4,71 %
Maximum error	28,26 %
Mean mapping degree (data)	0,428
Min mapping degree (data)	0,136
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

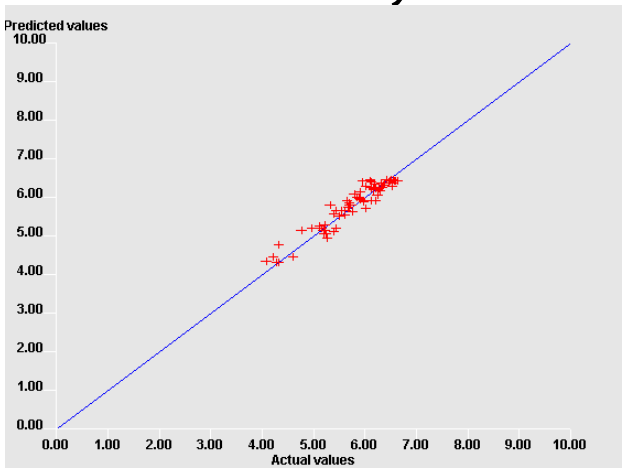


Correlation coefficient	0,858
Mean error (predicted - actual)	-0,06
Error standard deviation	0,786
Hamming's error	5,47 %
Maximum error	29,90 %
Mean mapping degree (data)	0,475
Min mapping degree (data)	0,100
Non mapped data count	99 (4 %)

Best models for whole sensory profile

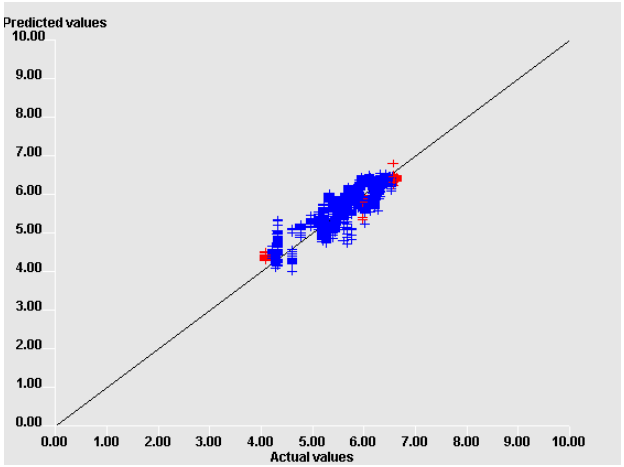
Whiteness ☺

Accuracy



Correlation coefficient	0,955
Mean error (predicted - actual)	0,044
Error standard deviation	0,187
Hamming's error	1,51 %
Maximum error	5,02 %
Mean mapping degree (data)	0,522
Min mapping degree (data)	0,245
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

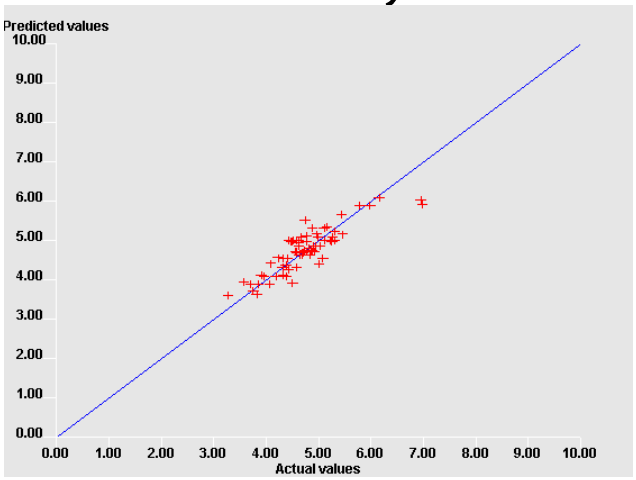


Correlation coefficient	0,913
Mean error (predicted - actual)	0,046
Error standard deviation	0,253
Hamming's error	2,06 %
Maximum error	10,28 %
Mean mapping degree (data)	0,569
Min mapping degree (data)	0,119
Non mapped data count	0 (0 %)

Best models for whole sensory profile

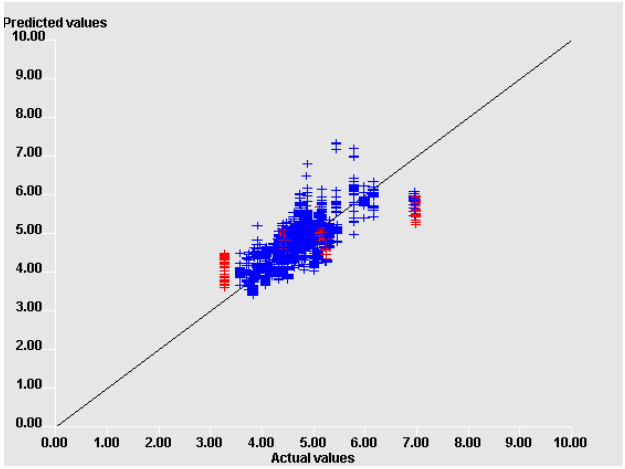
Color, Hue ☺

Accuracy



Correlation coefficient	0,866
Mean error (predicted - actual)	0,029
Error standard deviation	0,319
Hamming's error	2,38 %
Maximum error	10,53 %
Mean mapping degree (data)	0,371
Min mapping degree (data)	0,226
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

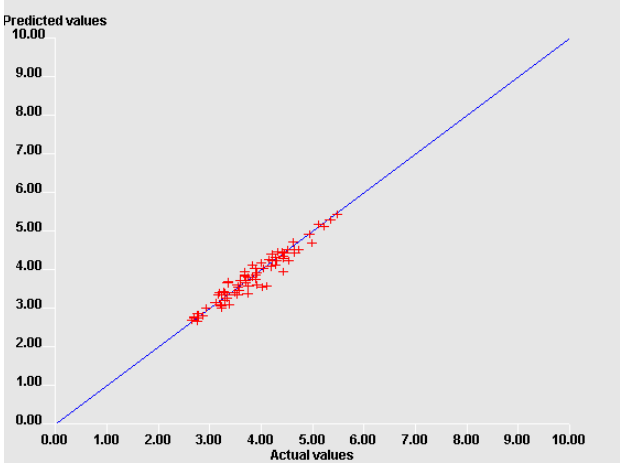


Correlation coefficient	0,750
Mean error (predicted - actual)	0,042
Error standard deviation	0,416
Hamming's error	3,13 %
Maximum error	19,26 %
Mean mapping degree (data)	0,399
Min mapping degree (data)	0,102
Non mapped data count	9 (0 %)

Best models for whole sensory profile

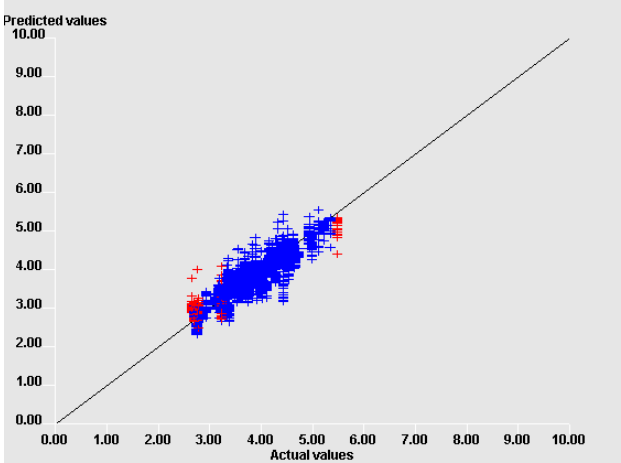
Color intensity ☺

Accuracy



Correlation coefficient	0,965
Mean error (predicted - actual)	-0,02
Error standard deviation	0,179
Hamming's error	1,37 %
Maximum error	5,16 %
Mean mapping degree (data)	0,384
Min mapping degree (data)	0,163
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

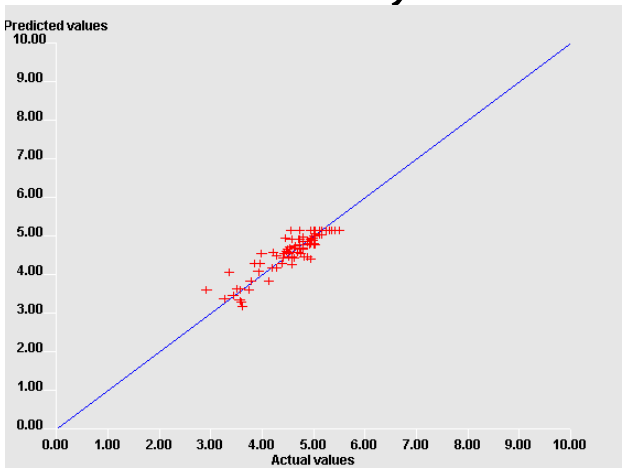


Correlation coefficient	0,906
Mean error (predicted - actual)	-0,01
Error standard deviation	0,290
Hamming's error	2,22 %
Maximum error	12,61 %
Mean mapping degree (data)	0,382
Min mapping degree (data)	0,103
Non mapped data count	1 (0 %)

Best models for whole sensory profile

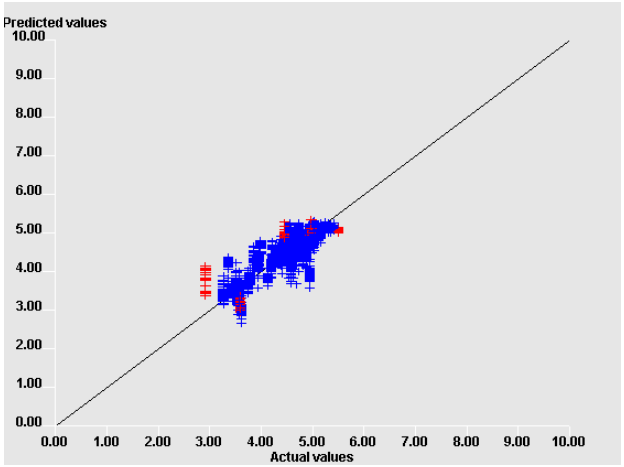
Mustard flavour ☺

Accuracy



Correlation coefficient	0,892
Mean error (predicted - actual)	0,022
Error standard deviation	0,256
Hamming's error	1,94 %
Maximum error	6,99 %
Mean mapping degree (data)	0,305
Min mapping degree (data)	0,162
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

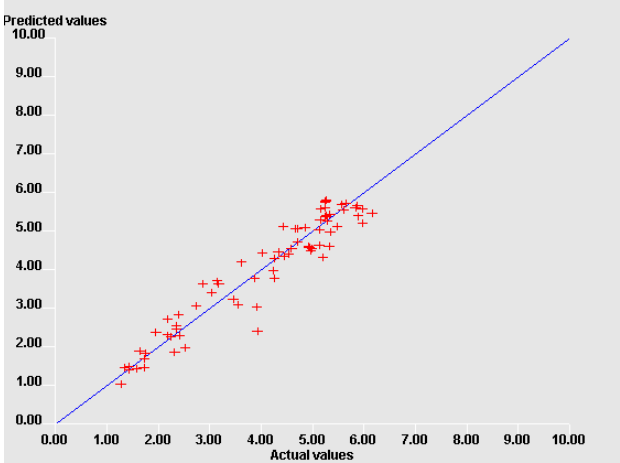


Correlation coefficient	0,815
Mean error (predicted - actual)	0,017
Error standard deviation	0,334
Hamming's error	2,51 %
Maximum error	13,61 %
Mean mapping degree (data)	0,305
Min mapping degree (data)	0,100
Non mapped data count	54 (2 %)

Best models for whole sensory profile

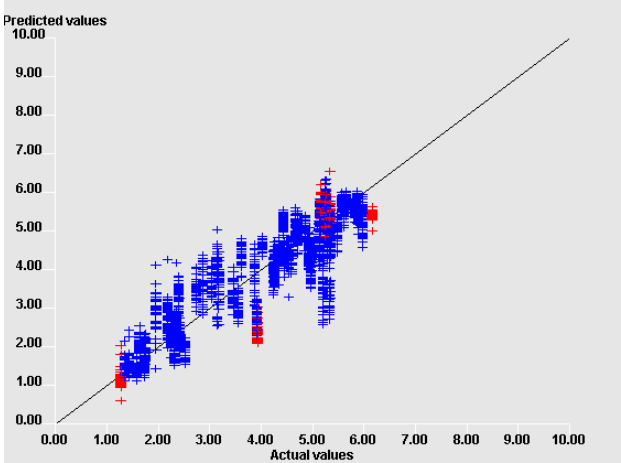
Acidic flavour ☺

Accuracy



Correlation coefficient	0,958
Mean error (predicted - actual)	-0,02
Error standard deviation	0,423
Hamming's error	3,28 %
Maximum error	15,22 %
Mean mapping degree (data)	0,354
Min mapping degree (data)	0,128
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

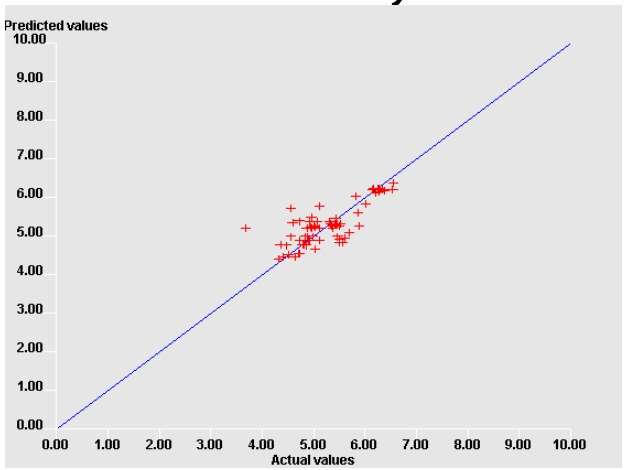


Correlation coefficient	0,909
Mean error (predicted - actual)	-0,03
Error standard deviation	0,625
Hamming's error	4,75 %
Maximum error	26,09 %
Mean mapping degree (data)	0,398
Min mapping degree (data)	0,101
Non mapped data count	201 (7 %)

Best models for whole sensory profile

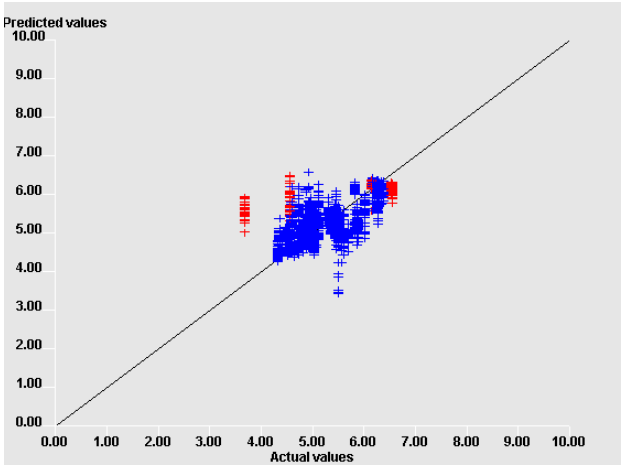
Sour flavour ☹

Accuracy



Correlation coefficient	0,804
Mean error (predicted - actual)	0,032
Error standard deviation	0,378
Hamming's error	2,60 %
Maximum error	15,30 %
Mean mapping degree (data)	0,379
Min mapping degree (data)	0,144
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

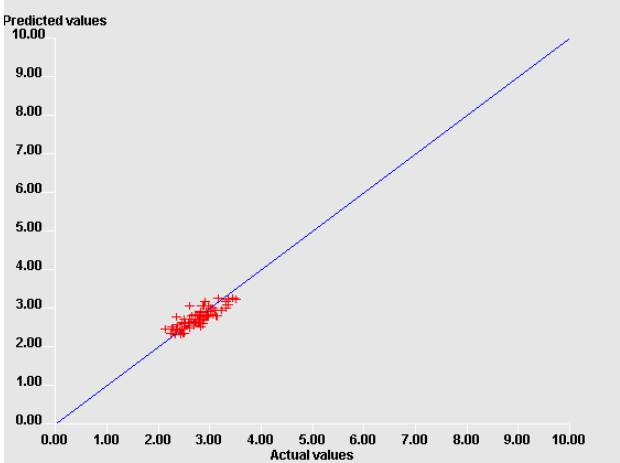


Correlation coefficient	0,691
Mean error (predicted - actual)	0,037
Error standard deviation	0,471
Hamming's error	3,30 %
Maximum error	22,60 %
Mean mapping degree (data)	0,374
Min mapping degree (data)	0,102
Non mapped data count	100 (4 %)

Best models for whole sensory profile

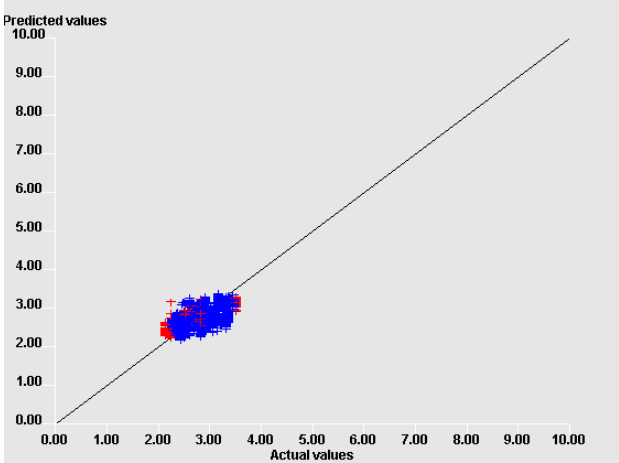
Sweetness ☹

Accuracy



Correlation coefficient	0,822
Mean error (predicted - actual)	-0,01
Error standard deviation	0,172
Hamming's error	1,38 %
Maximum error	4,53 %
Mean mapping degree (data)	0,513
Min mapping degree (data)	0,185
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

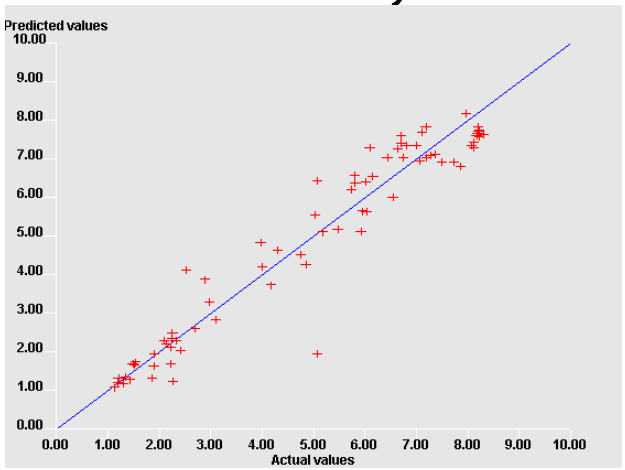


Correlation coefficient	0,538
Mean error (predicted - actual)	-0,02
Error standard deviation	0,263
Hamming's error	2,12 %
Maximum error	9,21 %
Mean mapping degree (data)	0,505
Min mapping degree (data)	0,110
Non mapped data count	2 (0 %)

Best models for whole sensory profile

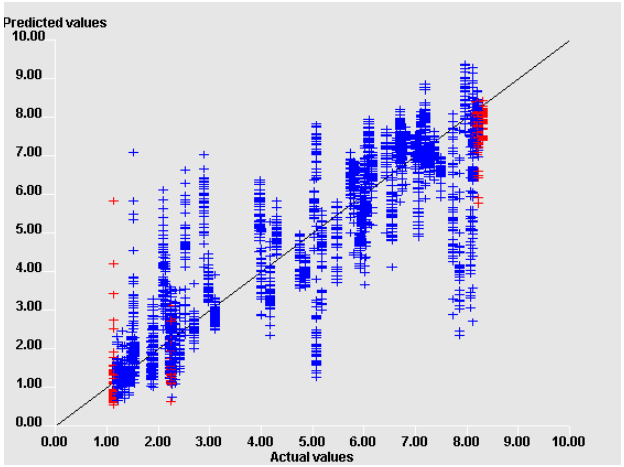
Fresh Flavour ☹

Accuracy



Correlation coefficient	0,963
Mean error (predicted - actual)	-0,03
Error standard deviation	0,667
Hamming's error	4,88 %
Maximum error	31,24 %
Mean mapping degree (data)	0,417
Min mapping degree (data)	0,108
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

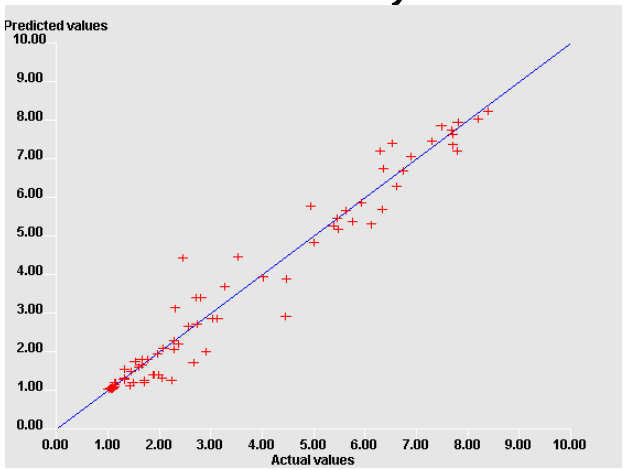


Correlation coefficient	0,878
Mean error (predicted - actual)	-0,01
Error standard deviation	1,189
Hamming's error	8,22 %
Maximum error	55,93 %
Mean mapping degree (data)	0,399
Min mapping degree (data)	0,101
Non mapped data count	66 (2 %)

Best models for whole sensory profile

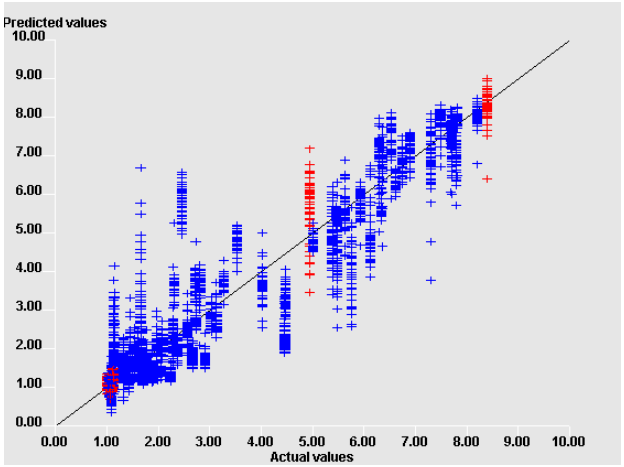
Rancid Flavour ☺

Accuracy



Correlation coefficient	0,978
Mean error (predicted - actual)	-0,04
Error standard deviation	0,504
Hamming's error	3,29 %
Maximum error	19,85 %
Mean mapping degree (data)	0,442
Min mapping degree (data)	0,167
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV

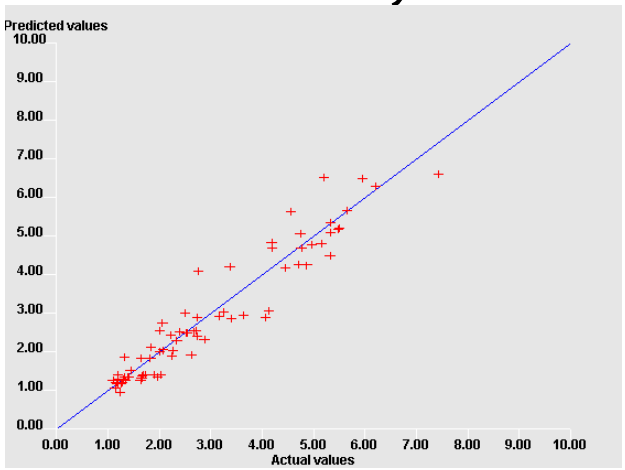


Correlation coefficient	0,936
Mean error (predicted - actual)	-0,03
Error standard deviation	0,858
Hamming's error	5,78 %
Maximum error	50,33 %
Mean mapping degree (data)	0,458
Min mapping degree (data)	0,100
Non mapped data count	57 (2 %)

Best models for whole sensory profile

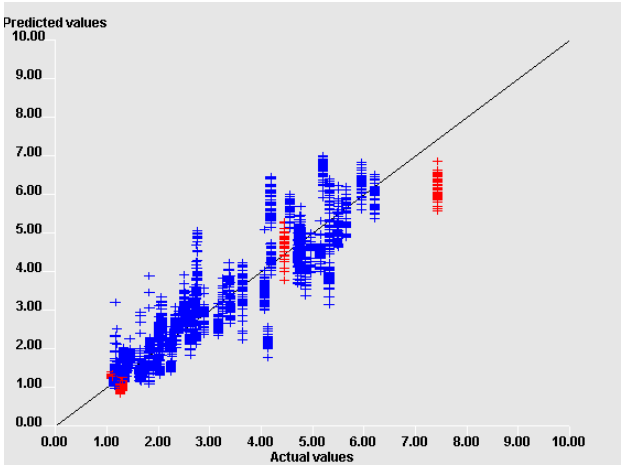
Off-Flavour ☺

Accuracy



Correlation coefficient	0,957
Mean error (predicted - actual)	-0,05
Error standard deviation	0,473
Hamming's error	3,44 %
Maximum error	13,33 %
Mean mapping degree (data)	0,331
Min mapping degree (data)	0,108
Non mapped data count	0 (0 %)

Monte Carlo 20%-CV



Correlation coefficient	0,925
Mean error (predicted - actual)	-0,01
Error standard deviation	0,622
Hamming's error	4,48 %
Maximum error	23,55 %
Mean mapping degree (data)	0,557
Min mapping degree (data)	0,105
Non mapped data count	27 (1 %)

Conclusions

- Some descriptors more difficult to model than others, but no descriptor proven impossible to model
- Linguistic rules form of the models allows experts to understand the underlying sensory phenomenon
- Models can be used to make direct predictions:
  "what would be at this date the degree of the dressing Mustard flavour, under these specific conditions of storage?"
- Models can be used to find optimal input values automatically (model inversion):
  "If I must store my dressing at ambient temperature, what would be the best packaging and light conditions to have strong Mustard flavour and light Rancid flavour after 5 months?"

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