Regularization approaches in sensory descriptive analysis

Applications to Kokumi-product development

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Sensometrics
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NPD-study コク味

- Goal of project
  1. Understand Japanese concept
  2. Identify koku-drivers in savoury/cullinary applications
  3. Support NPD to developed a koku-enhancing compound

- Sub-goal (method development)
  Develop strategies to
  - link koku to sensory data (difference tests, QDA)
  - deal with large datasets
  - improve interpretability

Kokumi

Koku = コク ＝ 濃香 ＝ thickness, complexity, depth and/or width
mi = 味 ＝ 味道 ＝ taste

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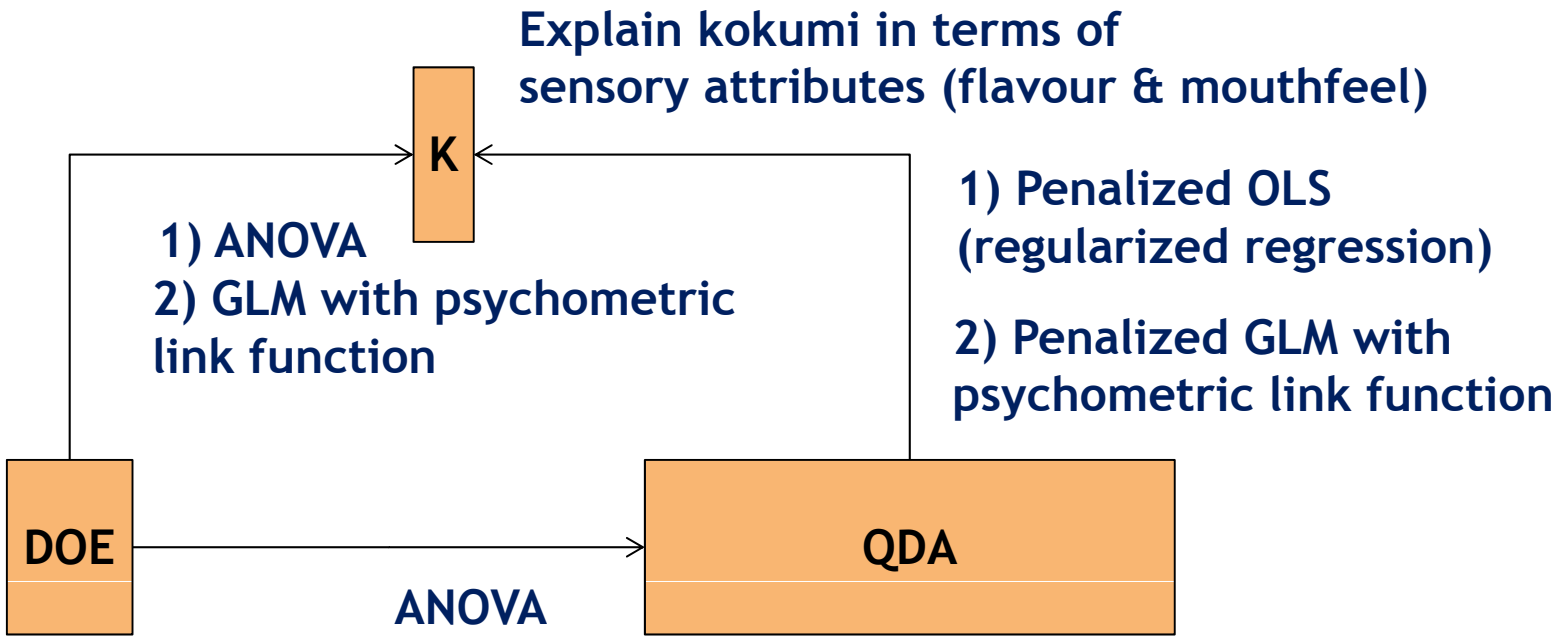
Project steps

- Evaluation in expert teams and QDA-panels (Japanese & Dutch)
- Interviews with Japanese cooks (n=80)
- Interviews with APAC consumers (Japan, China, Korea, n=600)
- Meat stew sensomics (NMR, GPC, LCMS, GCMS, QDA, etc.)
- YE-based reconstruction of koku-targeted flavour & mouthfeel
- Consumer tests: testing NPD samples against competition
- Lots of data – difficult to interpret – need for sparse methods both for regression and explorative analysis

Data & models



Alternatives

1) PLS/RR
   - greedy
   - developed for smooth spectra
2) GLM with psycho-lf. on PCA scores
   - more difficult to interpret

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Regularization

in multivariate regression

- **Multivariate regression**

$$y = \mathbf{X}\beta + \varepsilon$$

- **OLS minimizes**

$$\|y - \mathbf{X}\beta\|^2$$

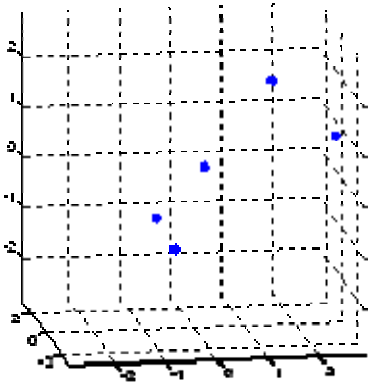
- **Solution**

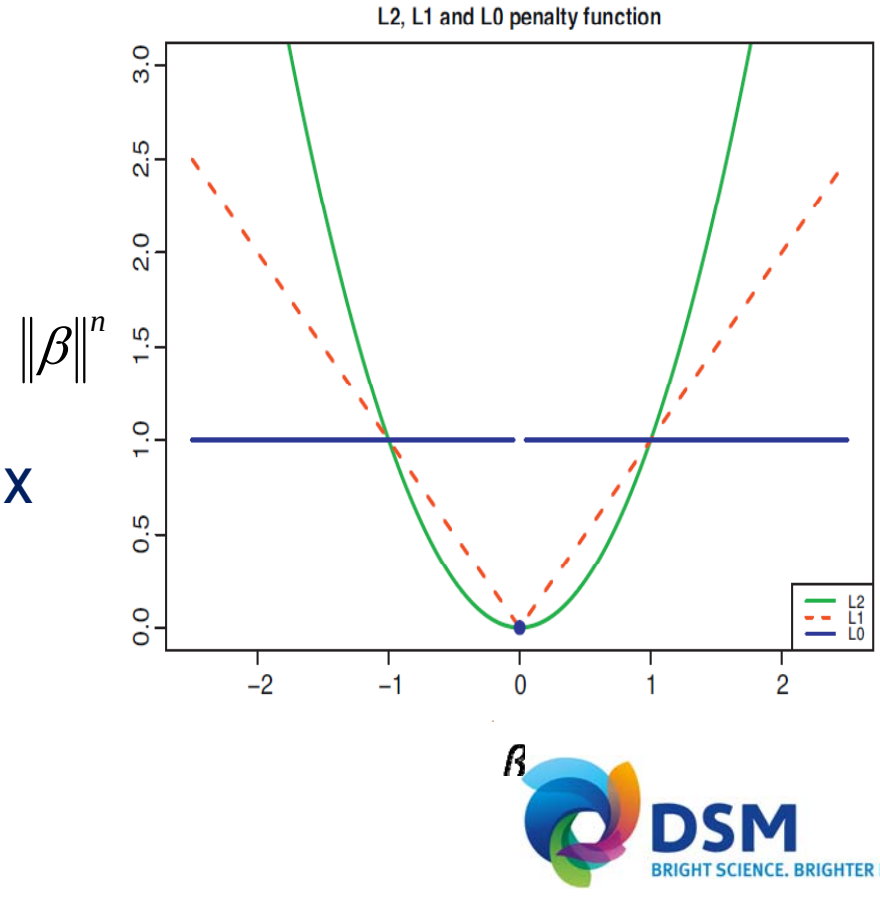
$$\beta = \left(\mathbf{X}^t\mathbf{X}\right)^{-1}\mathbf{X}^t y$$

- **Inversion problems for collinear X**

- **Solution:** restrict beta's

$$\|y - \mathbf{X}\beta\|^2 + \lambda\|\beta\|^n$$





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Regularization

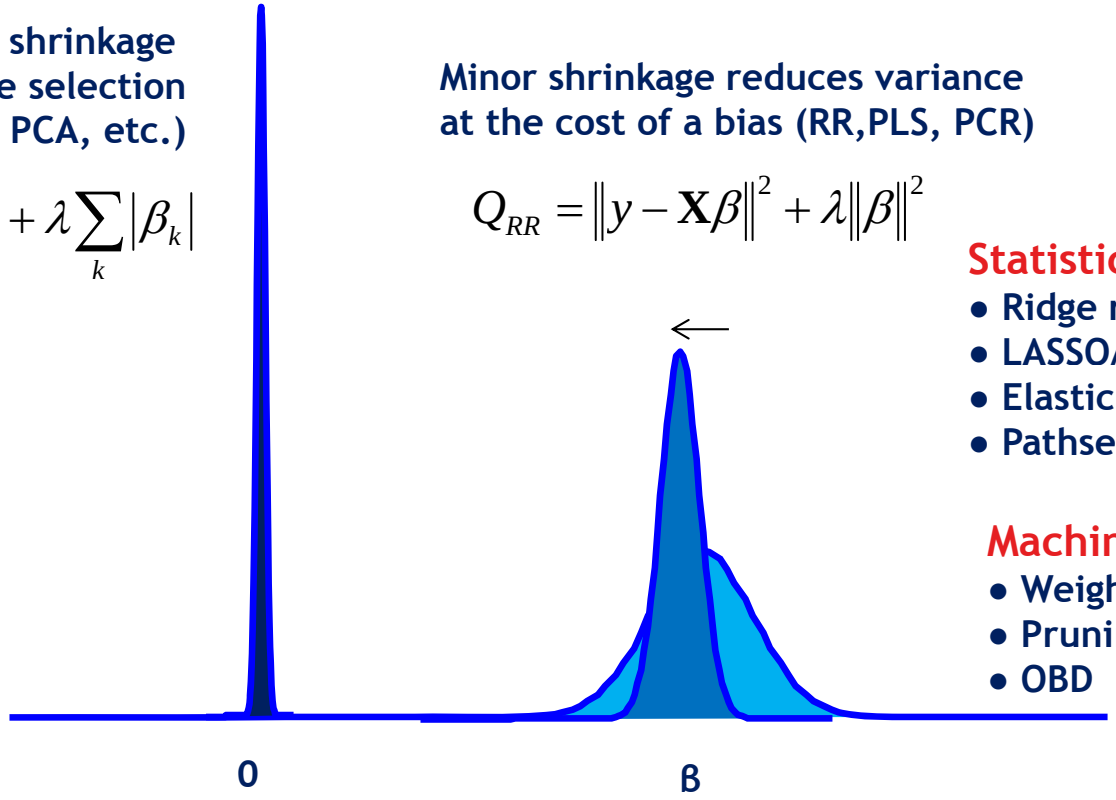
in multivariate regression

Heavy shrinkage brings variable selection (Sparse OLS, Sparse PCA, etc.)

$$Q_{L1} = \|y - \mathbf{X}\beta\|^2 + \lambda \sum_k |\beta_k|$$

Minor shrinkage reduces variance at the cost of a bias (RR,PLS, PCR)

$$Q_{RR} = \|y - \mathbf{X}\beta\|^2 + \lambda \|\beta\|^2$$



Statistics

- Ridge regression
- LASSO/ LARS
- Elastic net
- Pathseeker

Machine learning

- Weight decay
- Pruning
- OBD

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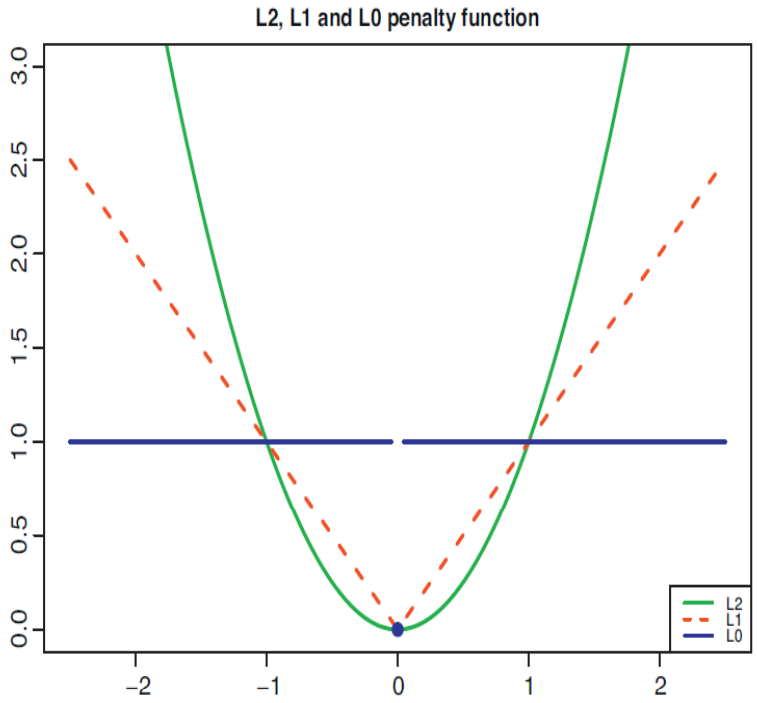
Regularization

in principal component analysis



- **PCA**

$$\hat{\mathbf{X}} = tp^{t}$$

$$Q_{PCA} = \left\| \mathbf{X} - tp^{t} \right\|^{2}$$

- **Issues:**
  - messy biplots
  - many variables (e.g. internal prefmapping, higher order QDA)
  - many objects (e.g. consumer studies)

- **Sparse PCA**
  - Shrink loadings (automatic attribute selection)

$$Q_{L2(p)} = \left\| \mathbf{X} - tp^{t} \right\|^{2} + \lambda \left\| p \right\|^{2}$$

$$Q_{L1(p)} = \left\| \mathbf{X} - tp^{t} \right\|^{2} + \lambda \sum_{j} \left| p_{j} \right|$$

$$Q_{L0(p)} = \left\| \mathbf{X} - tp^{t} \right\|^{2} + \lambda \sum_{j} \left(\left| p_{j} \right| > 0 \right)$$

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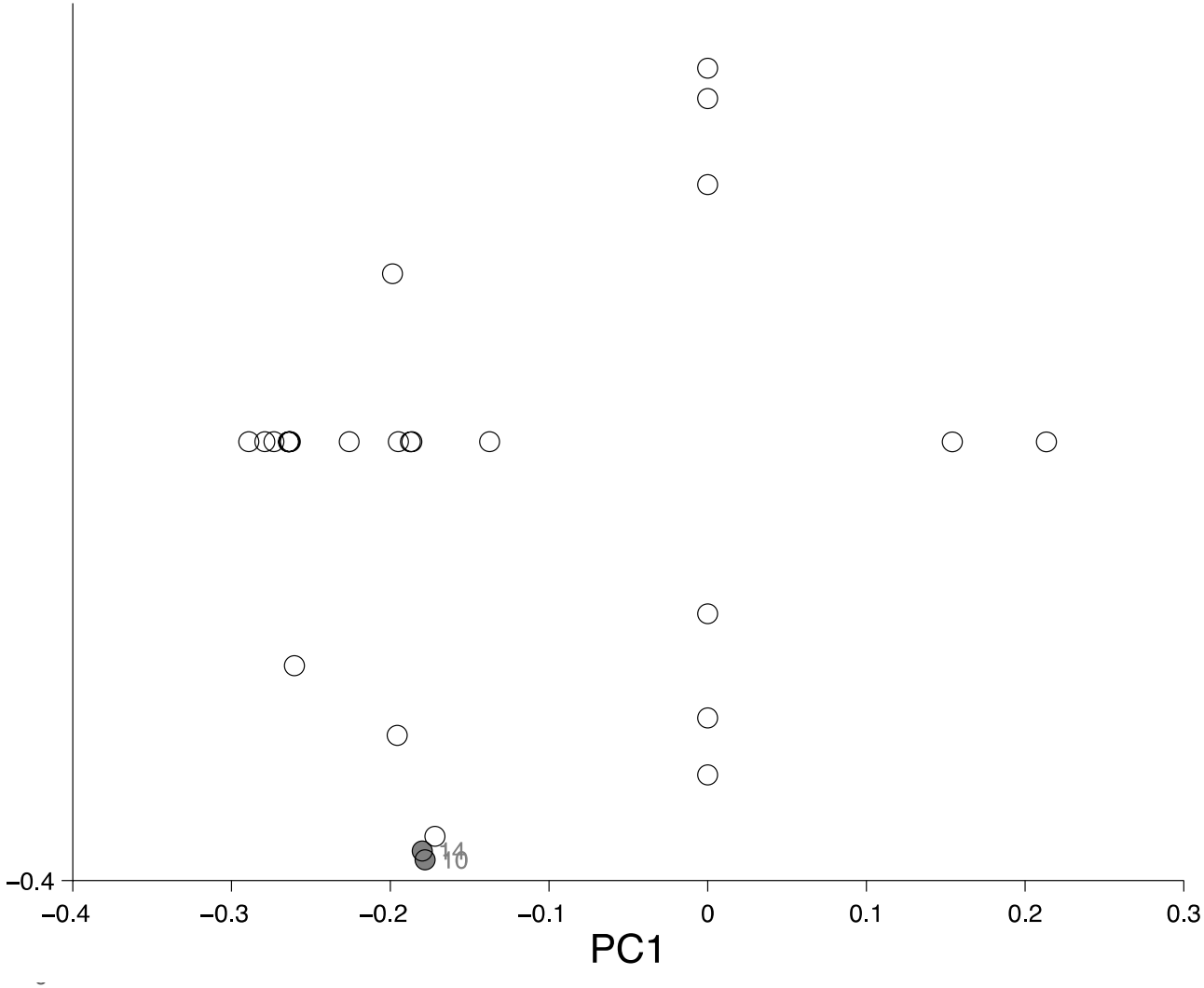
Regularization

in principal component analysis

Easier to interpret

- due to sparseness
- due to the fact that PC's get a meaning



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Regularization

in principal component analysis

- Can also be applied for sparse scores
- or penalization on scores and loadings simultaneously

This is called CoClustering*

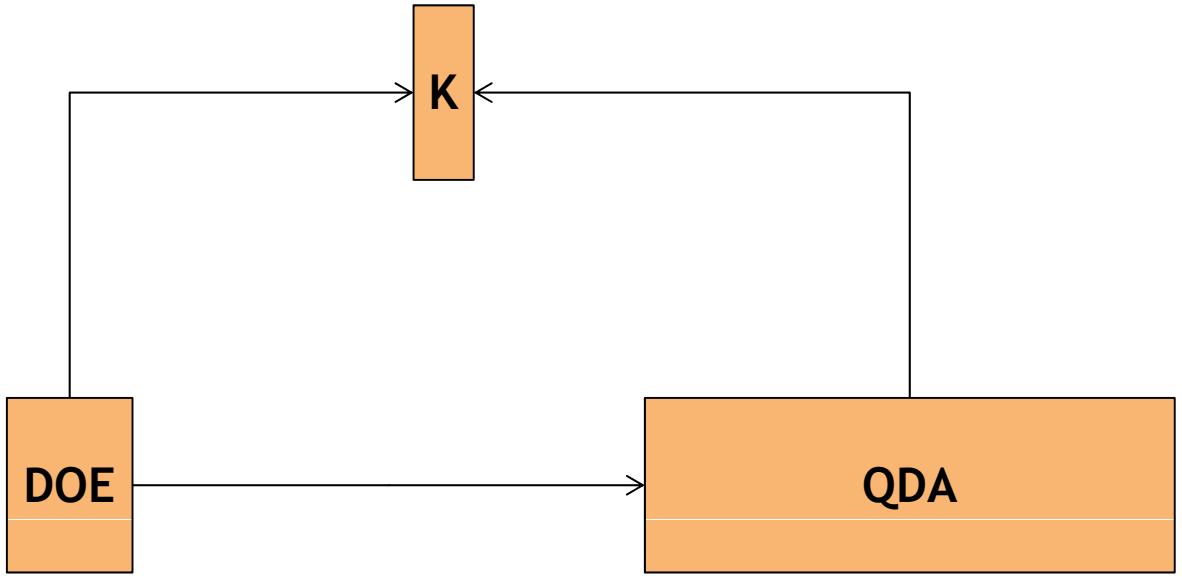
$$Q_{coclustering} = \left\| \mathbf{X} - tp^t \right\|^2 + \lambda \sum_i |t_i| + \mu \sum_j |p_j|$$

- method of choice when specific variables are related by specific groups of objects
  - contingency (COUNT) tables
  - CATA biplots (consumers x checked attributes)
  - sparse scoring data

** Bro, R., Papalexakis, E. E., Acar, E. and Sidiropoulos, N. D. (2012), Coclustering—a useful tool for chemometrics. J. Chemometrics, 26: 256–263.*

	Has eyes	Number of	Carnivor	Feather	Wings	Domestici	Eaten by C	>100kg	>2m	Breathe ur	Extinct	Dangerous	Life expect
Giraffe	1	4	0	0	0	0	0	1	1	0	0	0	30
Cow	1	4	0	0	0	1	1	1	1	0	0	0	15
Lion	1	4	1	0	0	0	0	1	0	0	0	1	15
Gorilla	1	4	0	0	0	0	0	1	0	0	0	1	30
Fly	1										0	0	0.1
Spider	1										0	0	1
Shark	1										0	1	50
House	0										0	0	100
Horse	1										0	0	15
Elephant	1										0	0	35
Mammoth	1										1	0	35
Sabre Tige	1										1	1	15
Pig	1										0	0	25
Cod	1										0	0	40
Eel	1										0	0	55
Jellyfish	1										0	0	0.7
Dolphin	1										0	0	30
Nemo	1										0	0	1
Shrimp	1										0	0	1
Dog	1										0	0	13
Cat	1										0	0	25
Fox	1										0	0	14
Wolf	1										0	1	18
Rabbit	1										0	0	9
Chicken	1										0	0	15
Eagle	1										0	0	55
Seagull	1										0	0	10
Blackbird	1	2	1	1	1	0	0	0	0	0	0	0	18
Bat	1	2	1	0	1	0	0	0	0	0	0	0	24
T. Rex.	1	4	1	0	0	0	0	1	1	0	1	1	40
Neanderth	1	4	1	0	0	0	0	0	0	0	1	0	50
Triceratops	1	4	1	0	0	0	0	1	1	0	1	1	30

Now some applications …



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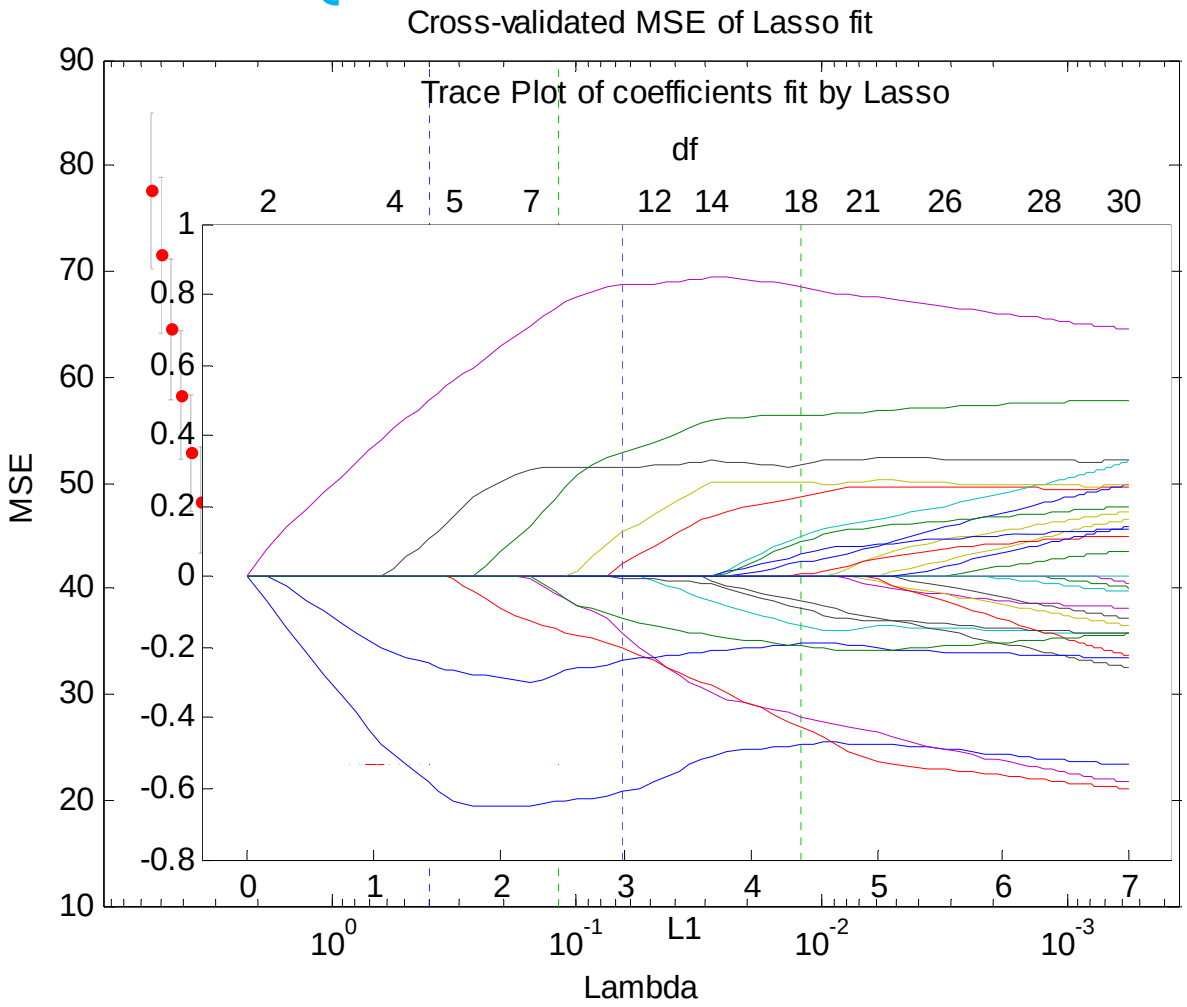
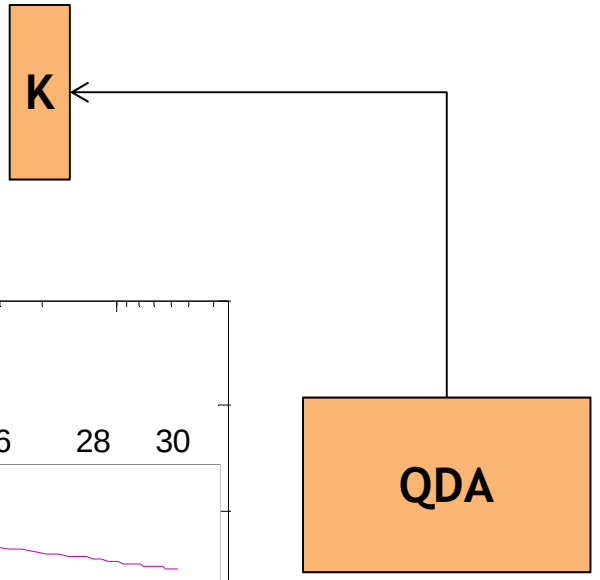
LASSO

koku versus QDA





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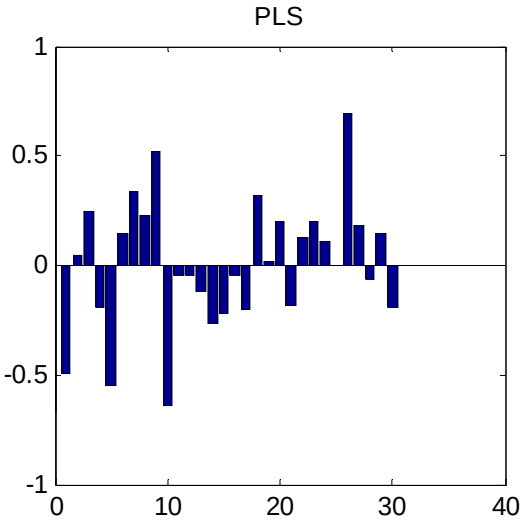
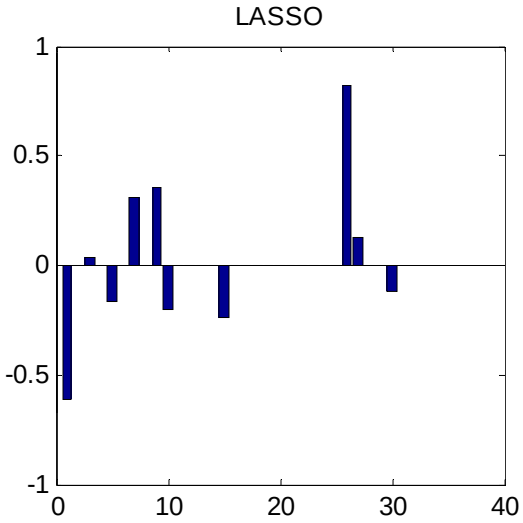
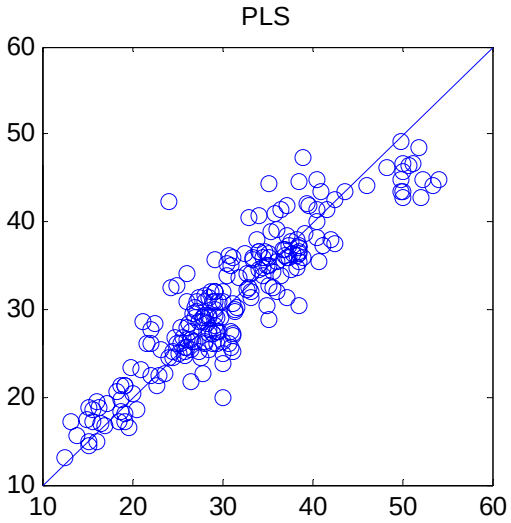
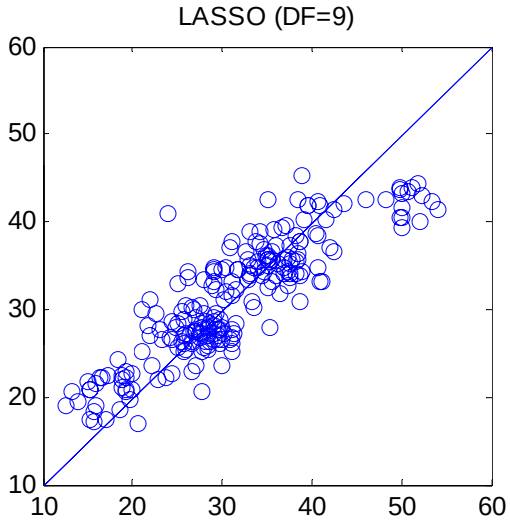
LASSO









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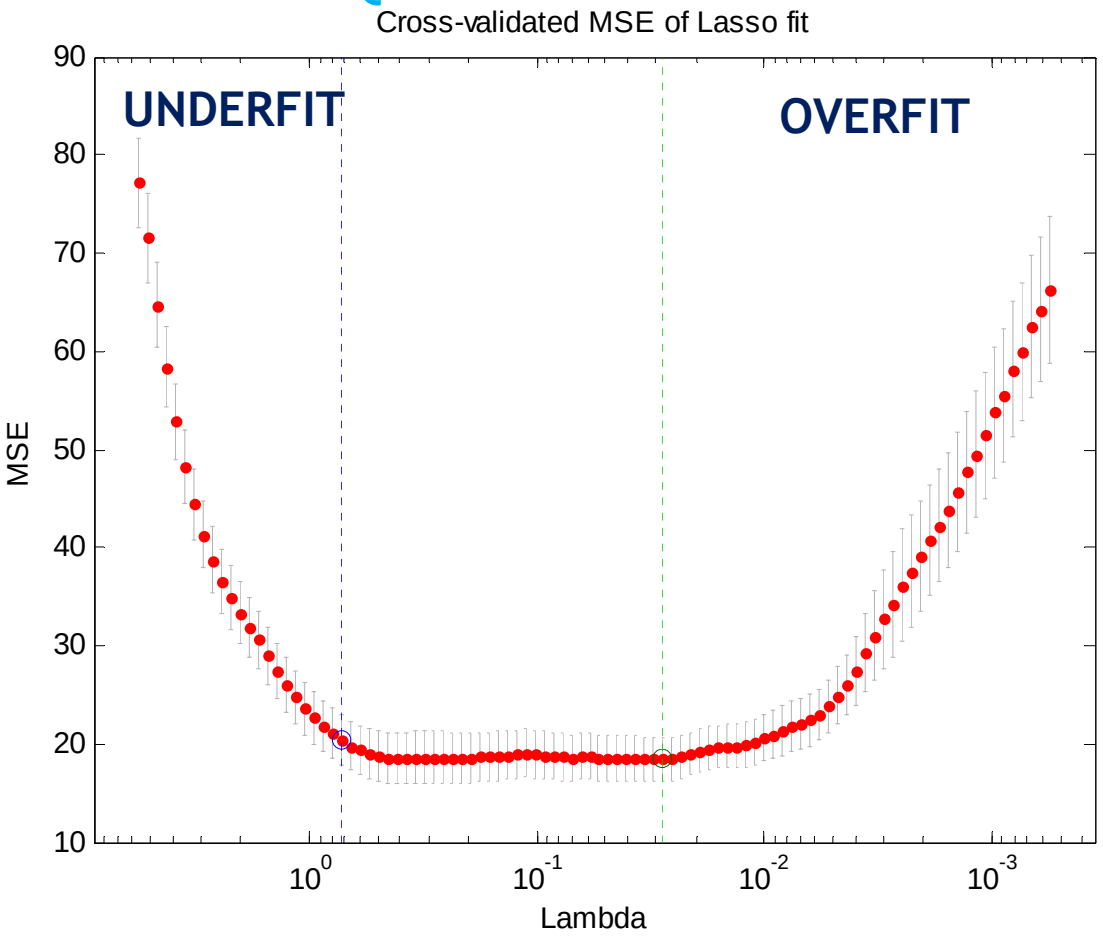
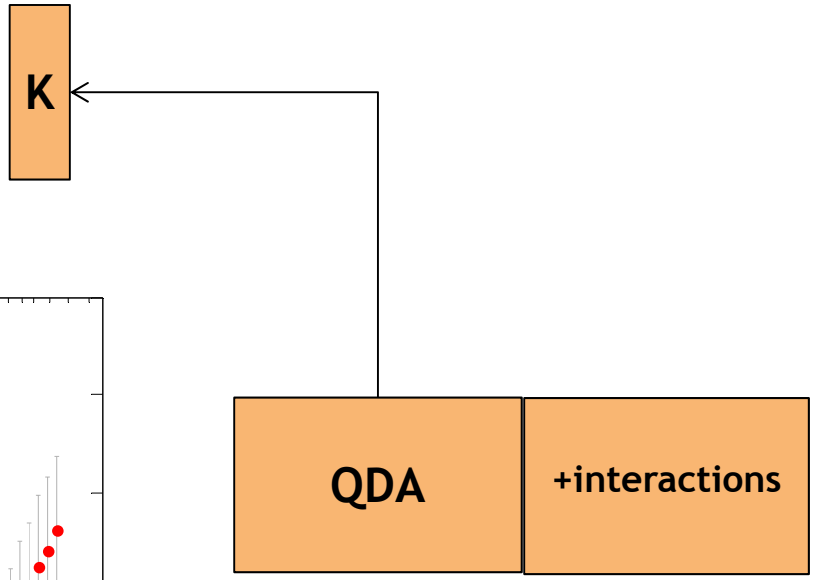
LASSO

koku versus QDA





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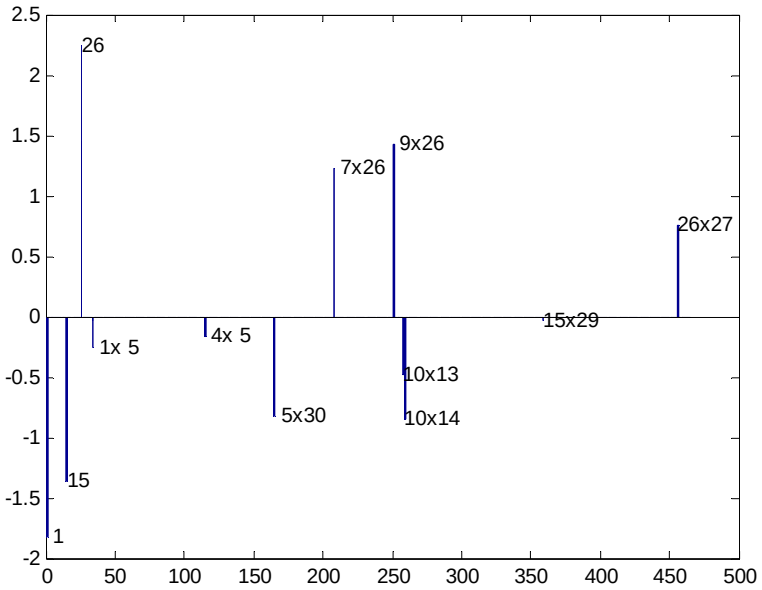

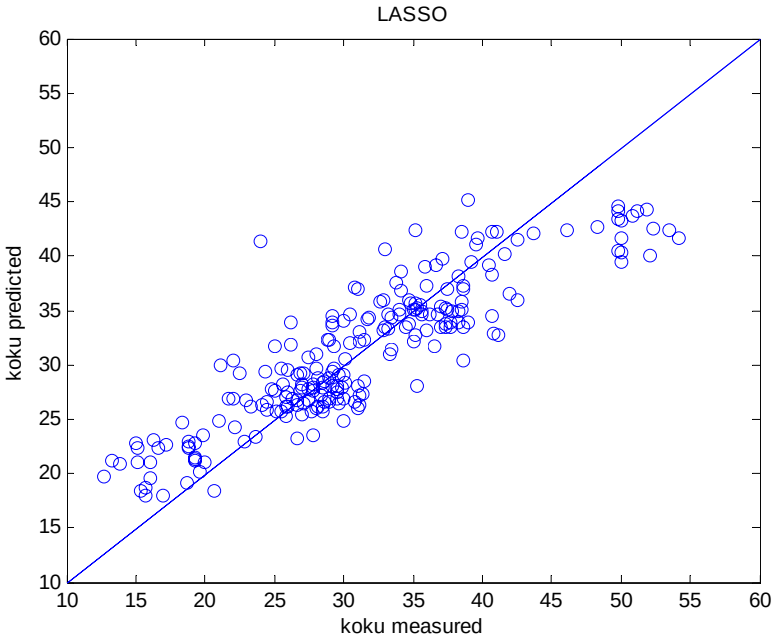

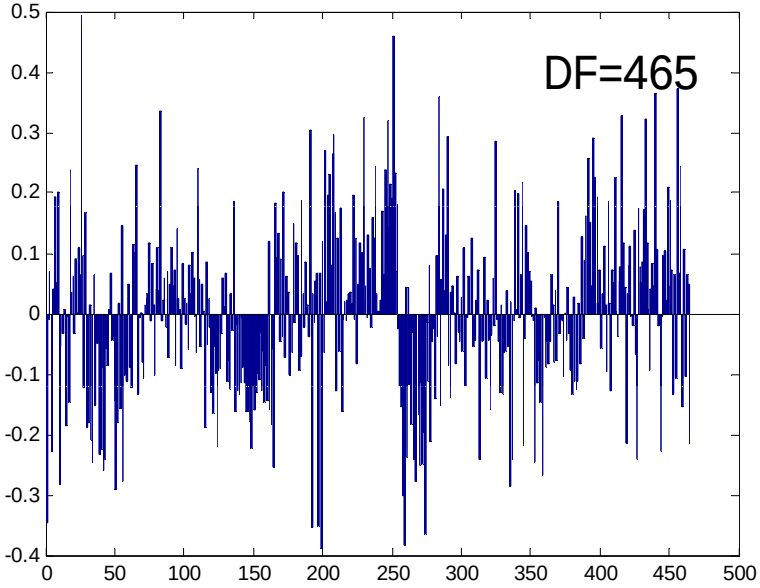

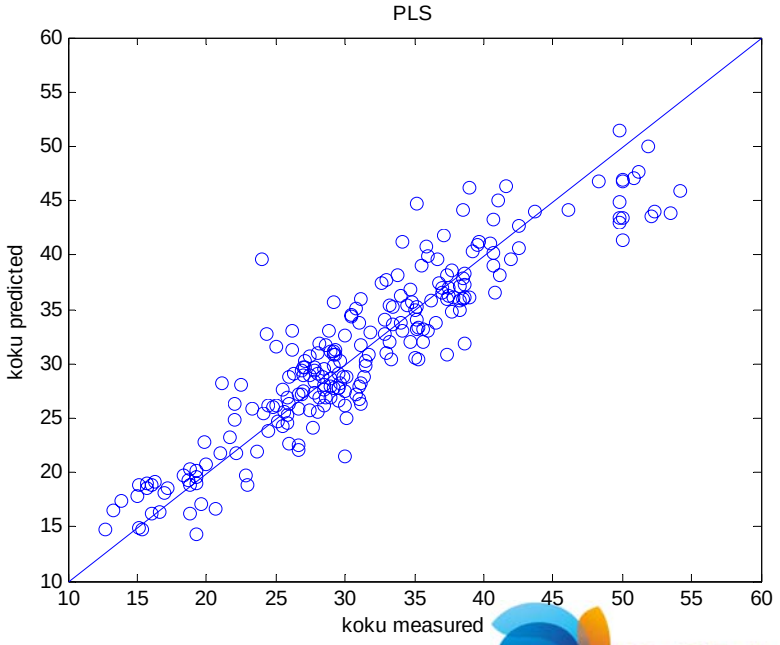

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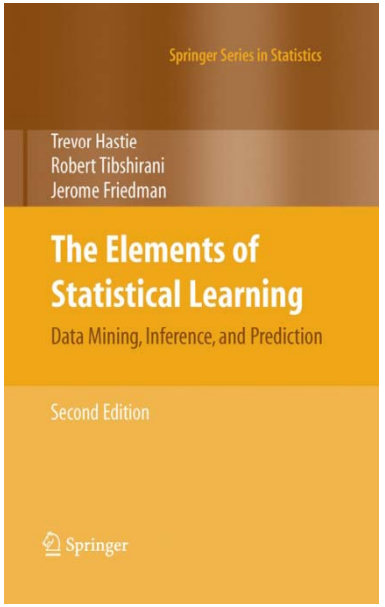
First conclusions



- LASSO selects a limited set of sensory attributes and interaction terms to explain kokumi with similar predictability compared to PLS
- But, LASSO improves interpretation (variable selection)
- PLS overfits (not demonstrated here)
- PLS (and RR) do not handle mega/multivariate sensory data well
  - eager to overfit
  - seeks correlated coefficients*

** Hastie, T., Tibshirani, R., Friedman, J. 'The elements of statistical learning'. Springer series in Statistics. Page 83*

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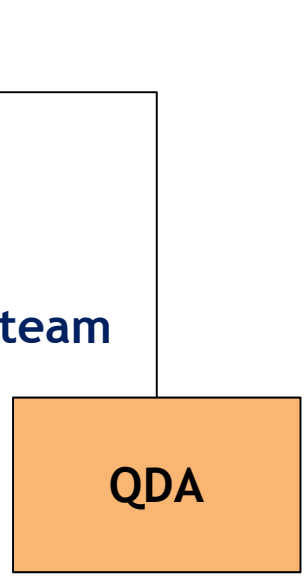
LASSO-GLM

MSG dose-response analysis



- Purpose: model umami perception from an EXPERT team as a function of QDA attributes with trained panelists
- EXPERT team (n=6) used 3AFC (2reps)
- QDA panel (n=14) (no umami in attribute list)
- MSG series (0, 0.12, 0.24, 0.36, 0.48, 0.60 percent)
- Applied in beef bouillon
- Proportion correct odds were modeled with GLM as function of MSG dosage and QDA attributes
- GLM model was organized with a 3AFC-psychometric link function and L1 penalty

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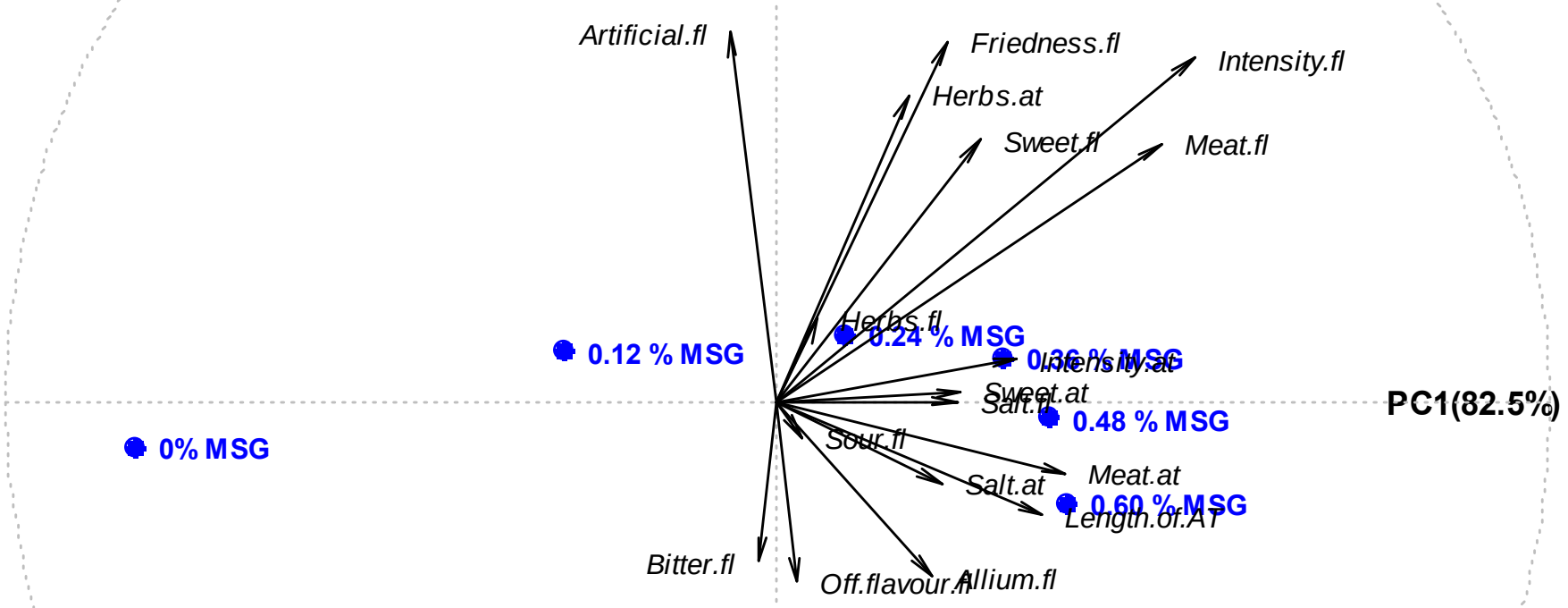
What about the panel?



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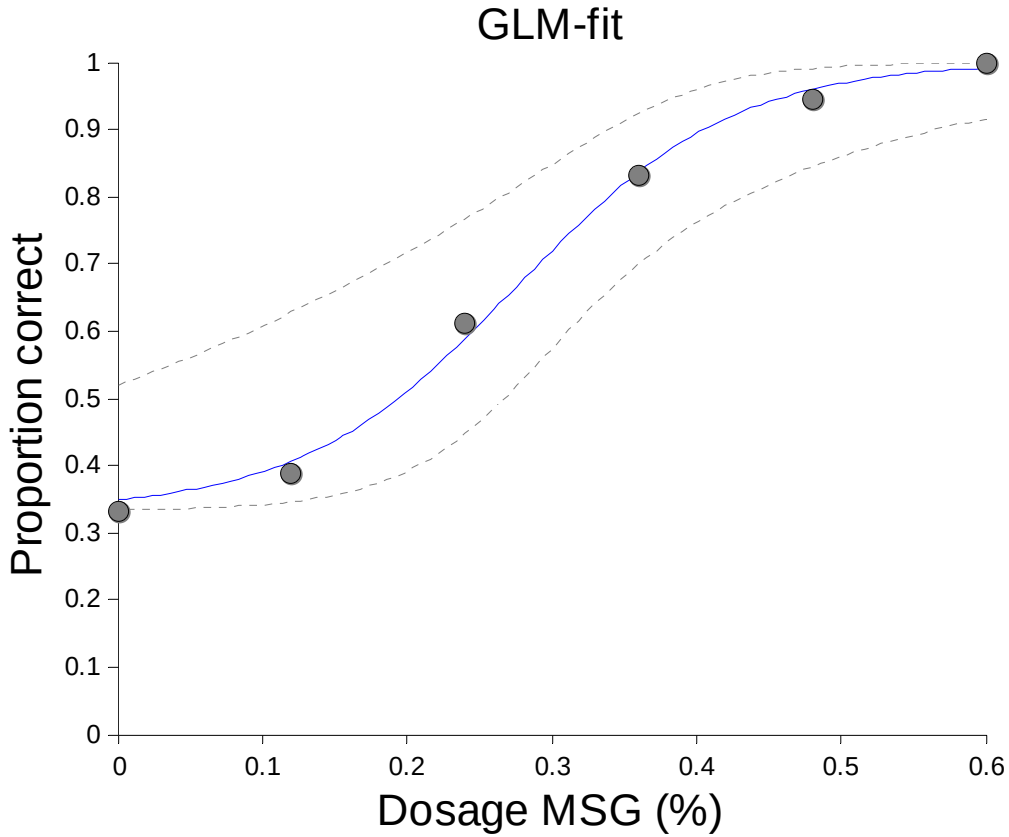
What about the experts?



Treatments in beef bouillon	Trials	Successes
'0.24 % MSG'	18	8
'0% MSG'	18	6
'0.36 % MSG'	18	15
'0.12 % MSG'	18	6
'0.60 % MSG'	18	18
'0.48 % MSG'	18	16

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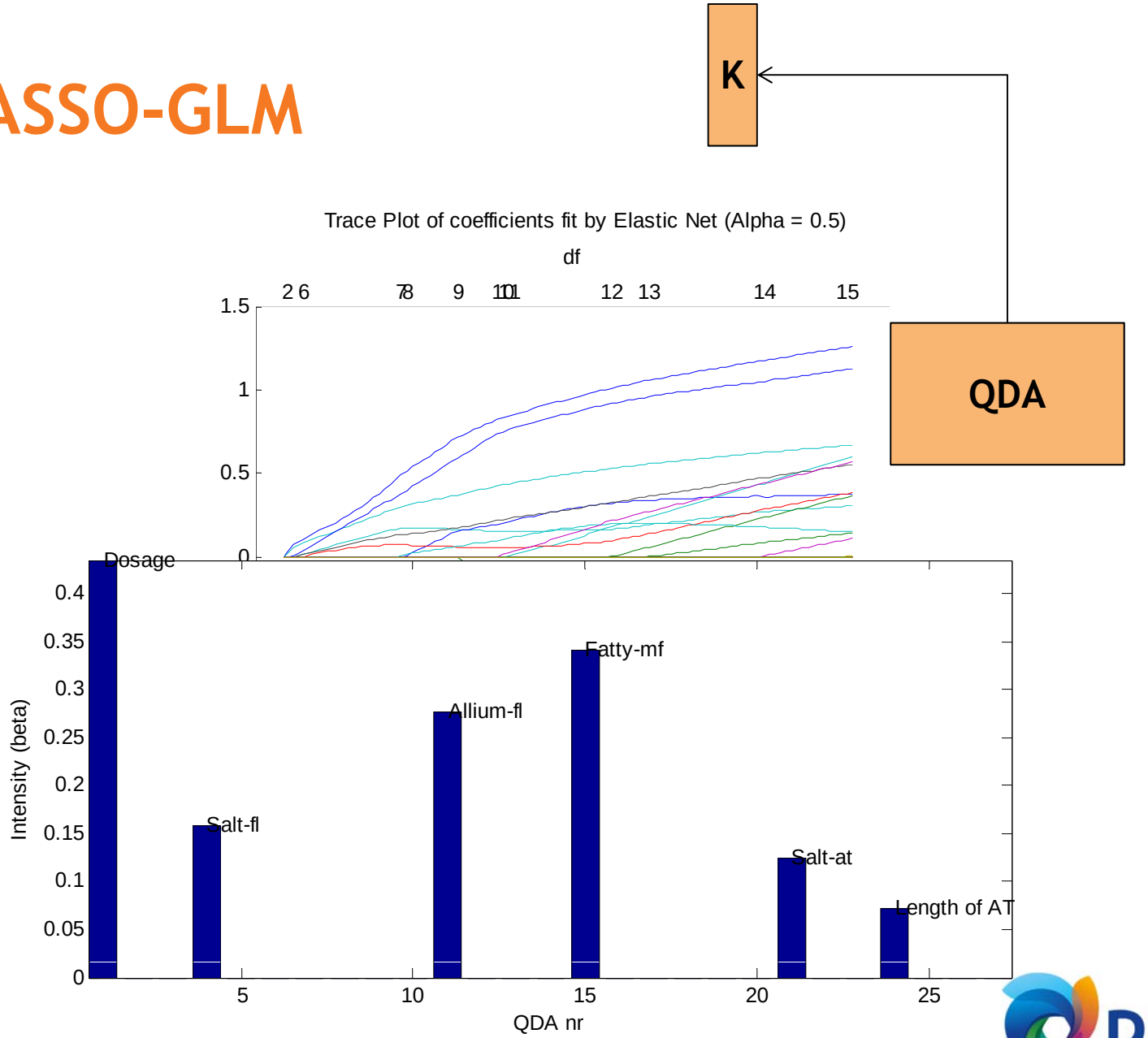
LASSO-GLM



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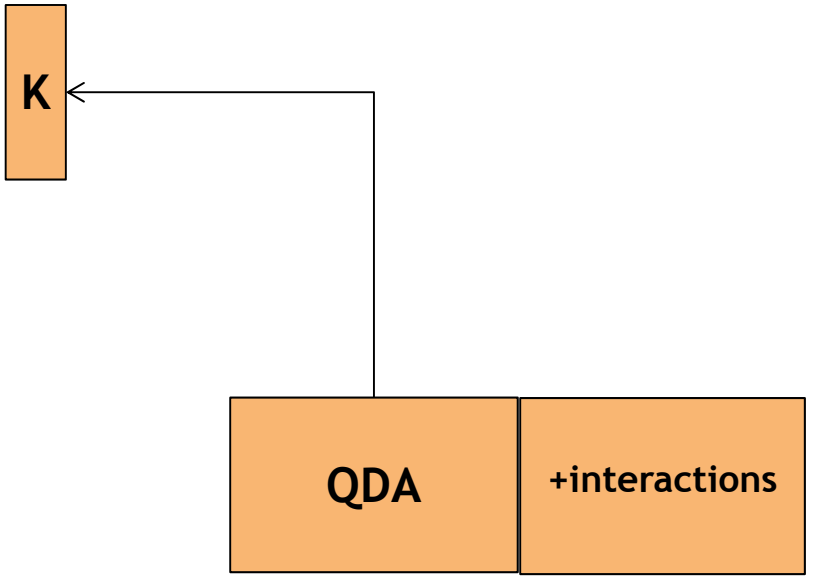
LASSO-GLM



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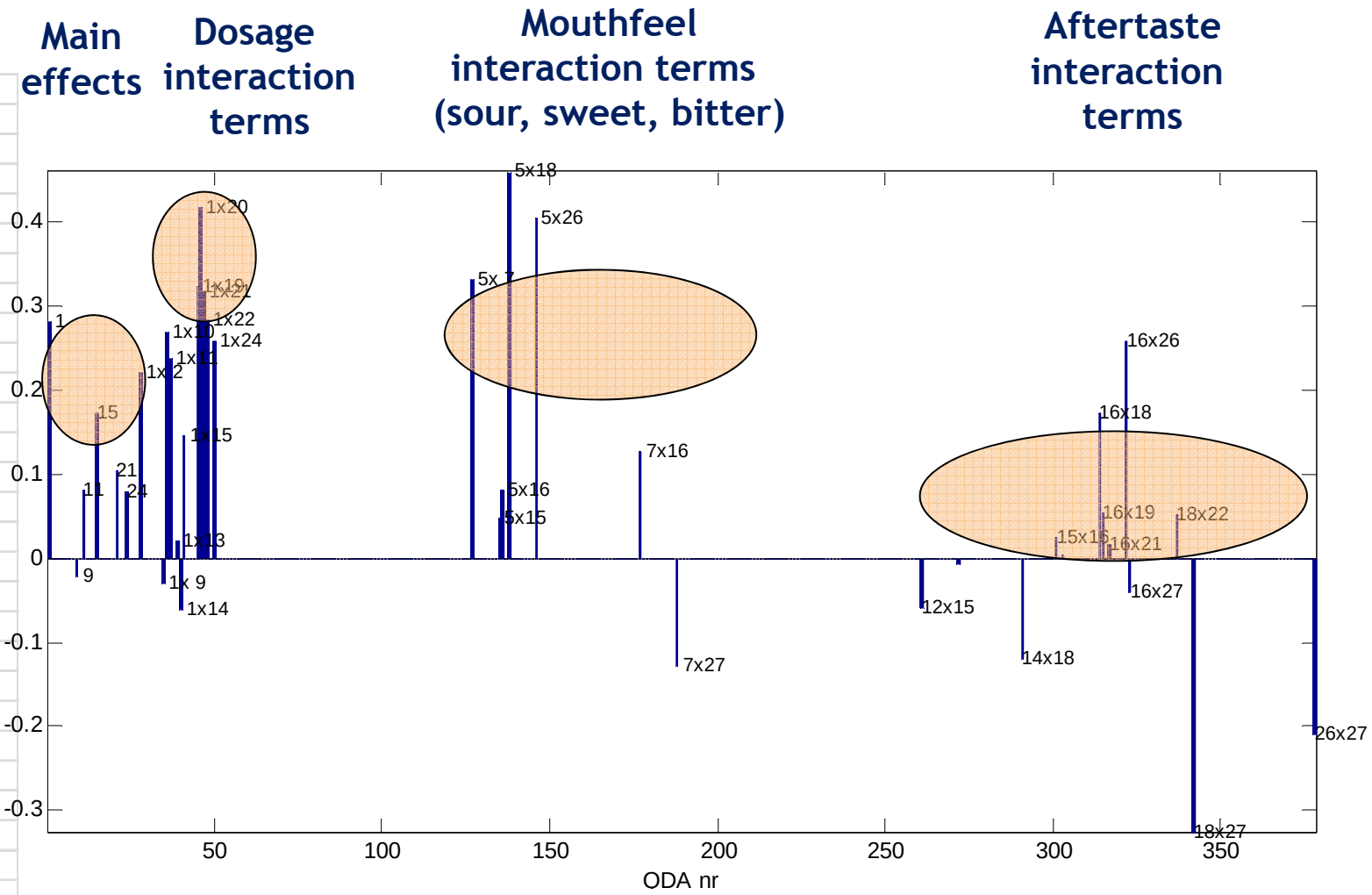
LASSO-GLM

NR	Attribute
1	'Dosage'
2	'Intensity-fl'
3	'Friedness-fl'
4	'Salt-fl'
5	'Sour-fl'
6	'Sweet-fl'
7	'Bitter-fl'
8	'Herbs-fl'
9	'Artificial-fl'
10	'Meat-fl'
11	'Allium-fl'
12	'Off flavour-fl'
13	'Fullness-mf'
14	'Pungent-mf'
15	'Fatty-mf'
16	'Rough-mf'
17	'Porridge-mf'
18	'Grainy-mf'
19	'Intensity-at'
20	'Sweet-at'
21	'Salt-at'
22	'Meat-at'
23	'Herbs-at'
24	'Length of AT'
25	'Fatty-af'
26	'Astringent-af'
27	'Tingling-af'



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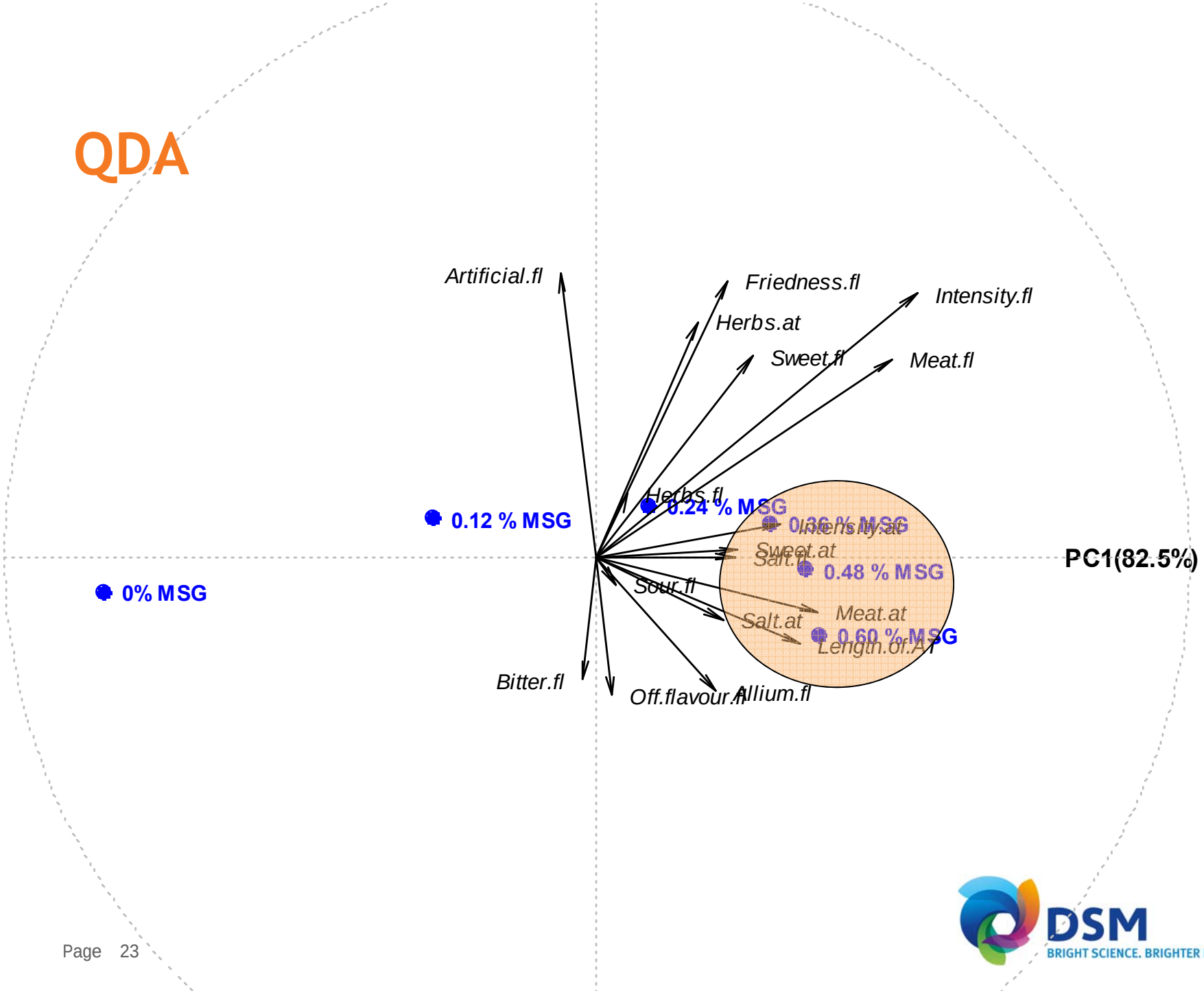
QDA



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Take home messages / conclusion

- Regularization is a powerful concept that enables
  - stabilization (RR)
  - sparseness (variable selection in PCA in OLS)
  - improved interpretability
  - improved predictability (for unseen data)
- Other types of restrictions (i.e. other than L_n) can be implemented as well
  - roughness penalties for smoothness (Smooth PCA)
  - dispersion penalties (clustering)
  - m-univariate regression (using correlation in y) (applications in shelf life analysis)

Thank you for your attention!

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