Quadratic PLS applied to external preference mapping

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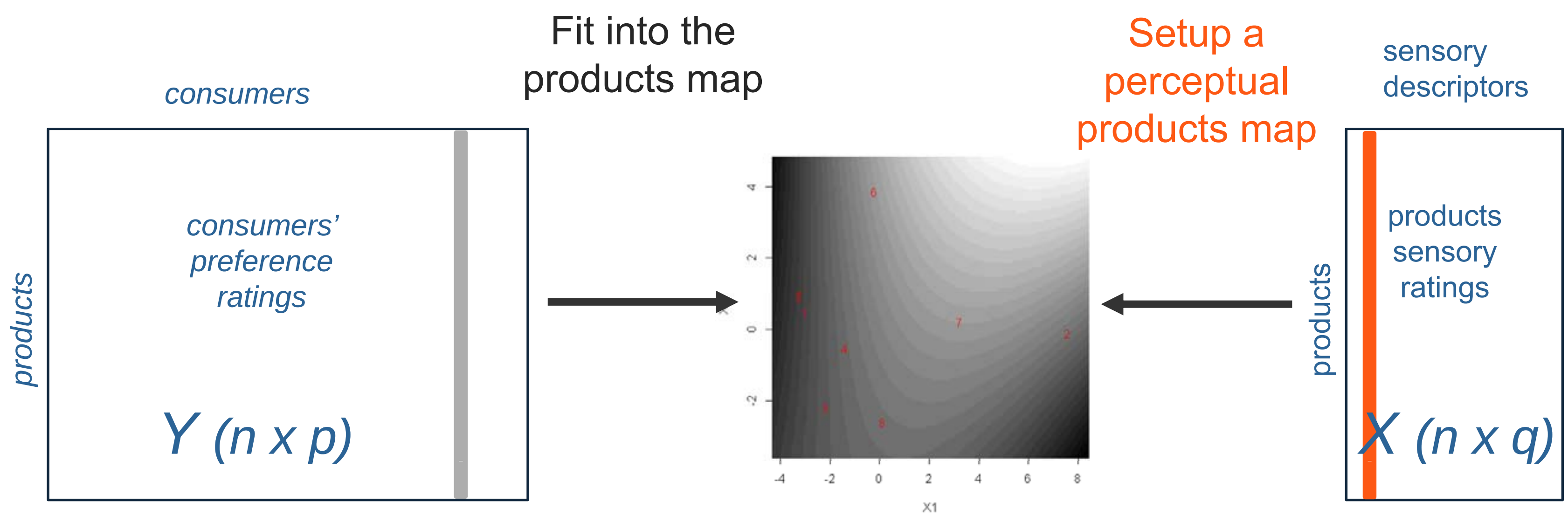
Context of Preference Mapping:

- relate data on consumers' preference to information on products
- identify attributes drivers of liking

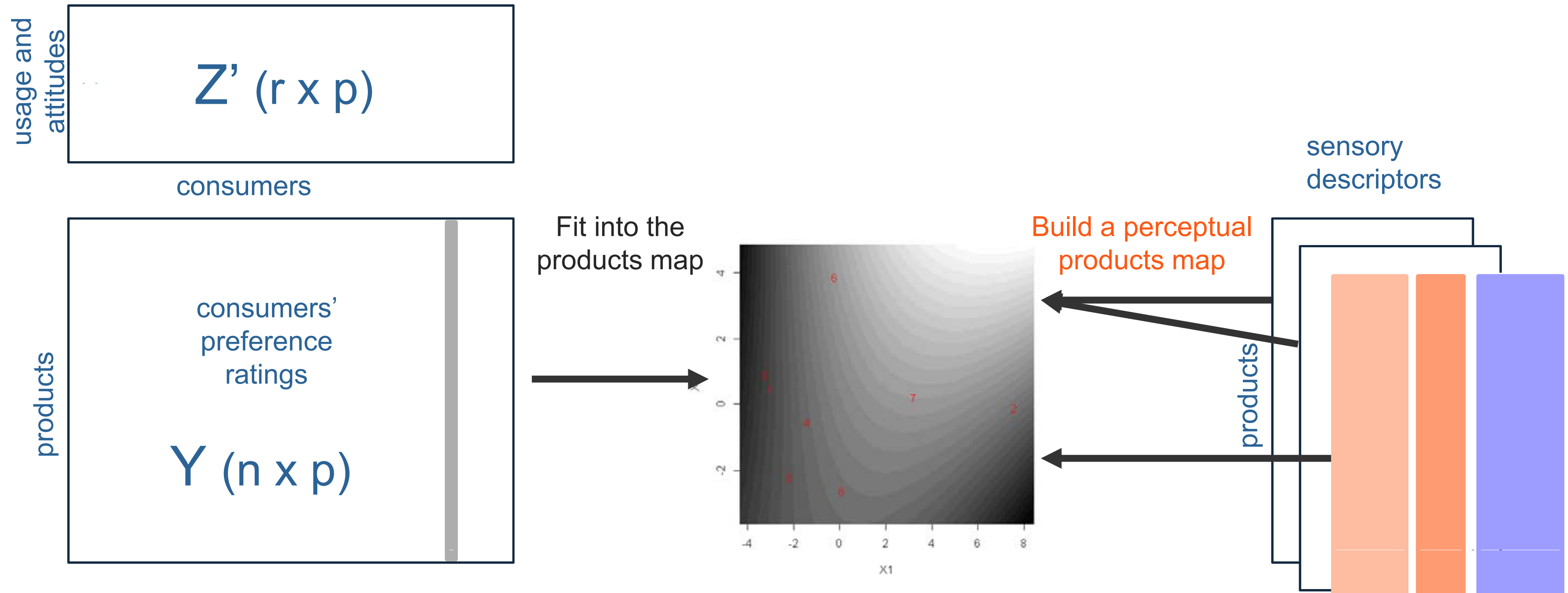
Usual implementation of external preference mapping:



Preference mapping

Extension to:

- sensory descriptors as a single consensus data table vs multiple data blocks vs multiway data
- information on consumers with a L-shaped data structure

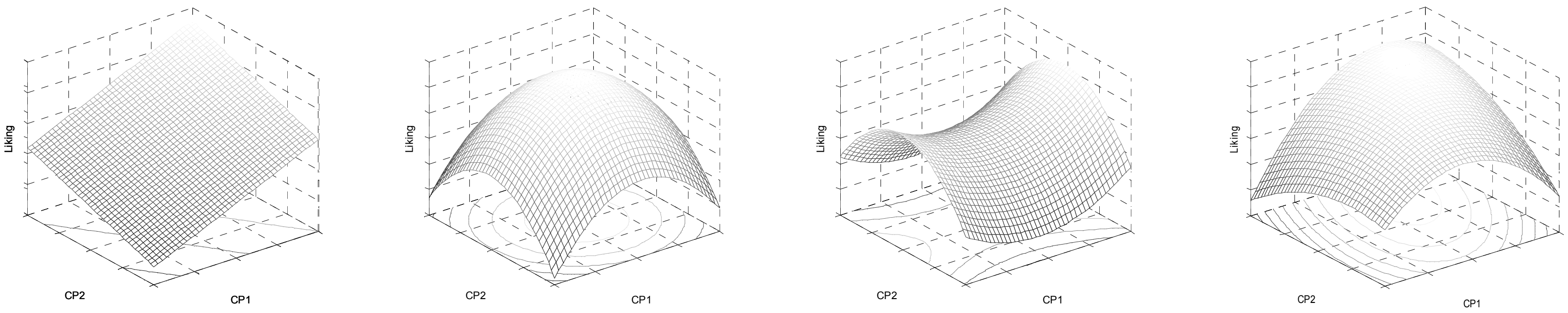


See Dijksterhuis & al. (2005) ; Lengard & al. (2006) ; Endrizzi & al. (2010) ; Mage & al. (2012).

Preference mapping

Adapt model to fit:

- vectorial vs polynomial models



Setting up of the products perceptual map:

- use of PCA vs PLS

Plan

- Models of Quadratic PLS
- Extension of Hoskuldsson's approach to several Y : QPLS2
- α - Regularization of QPLS2
- Application to Preference Mapping : The Coffee dataset
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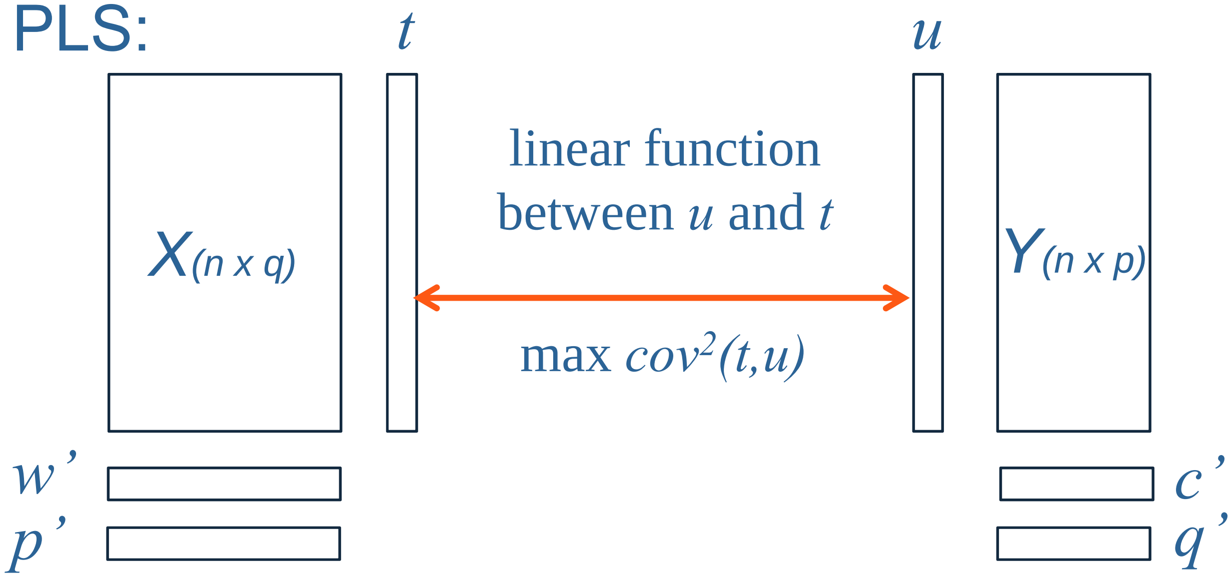
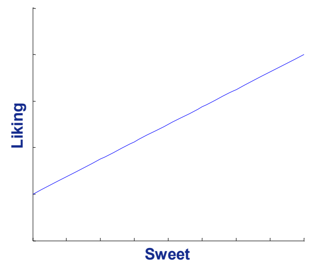
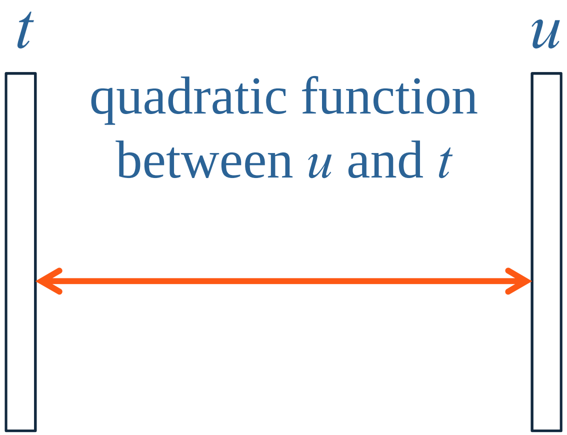
Models of Quadratic PLS

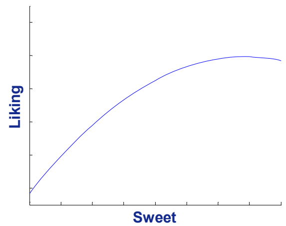
From PLS:





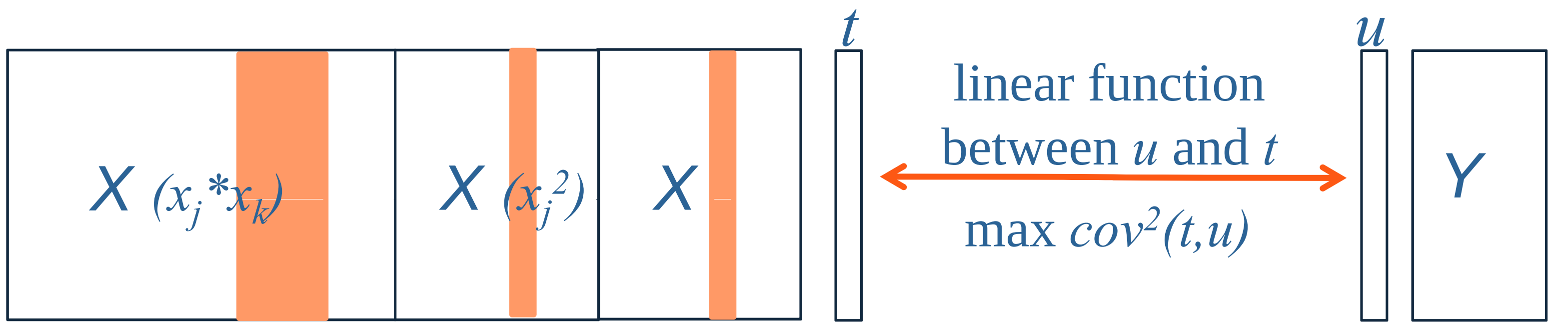
To quadratic PLS:



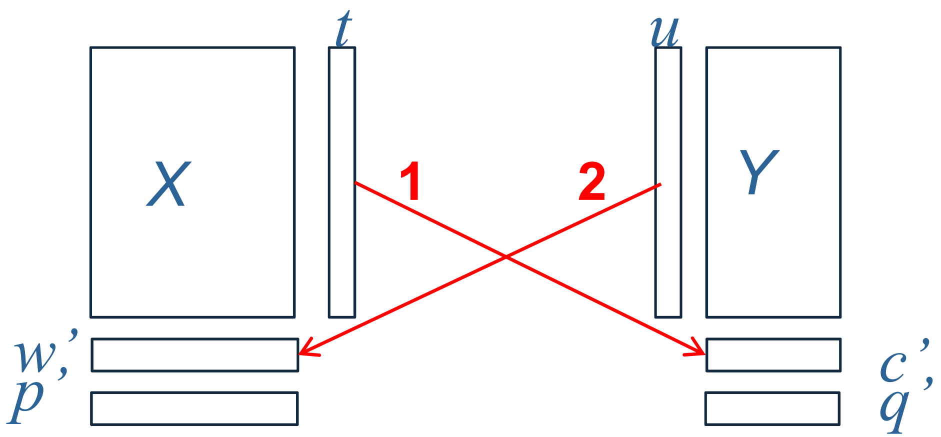


Models of Quadratic PLS

Gnanadesikan (1977), Wold & al. (1984), …



Wold & al. (1989), Baffi, Martin and Morris (1999)



1. **Estimate *c* by a quadratic regression of u on t**
2. **Update *w* by a Newton-Raphson-like linearization of the quadratic inner relation estimated by linear PLS**

Models of Quadratic PLS : Höskuldsson's approach

Höskuldsson (1992) extends the PLS1 criterion with the quadratic and interactions terms.

At step h, he seeks to maximize:

$$\operatorname{cov}^2(y,t_h)+\operatorname{cov}^2(y,t_h^2)+\operatorname{cov}^2(y,t_h t_1)+\ldots+\operatorname{cov}^2(y,t_h t_{h-1})$$

given $t_1, \ldots, t_{h-1}$ already known, and $t_h=X_{h-1}w_h$ with $\|w_h\|=1$.

On the basis of this criterion, Verdun & al. (2012) have proposed a revision of the original algorithm in order to guarantee convergence and optimality.

This latter one is extended in the case of QPLS2.

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Extension of Hoskuldsson's approach to several Y: QPLS2

The criterion can be modified to handle the case where Y has several variables.

At a step *h*, the algorithm seeks a component $u_h = Y_{h-1} c_h$ and a component $t_h = X_{h-1} w_h$ that maximise:

$$\operatorname{cov}^2(u_h, t_h) + \operatorname{cov}^2(u_h, t_h^2) + \operatorname{cov}^2(u_h, t_h t_1) + \ldots + \operatorname{cov}^2(u_h, t_h t_{h-1})$$

Extension of Hoskuldsson's approach to several Y: some limitations

The criterion uses the covariance between u on the one hand, and t and t^2 on the other hand. These variables can be at very different scale levels.

If t^2 variance is large compared to the variance of t, the objective criterion will be dominated by t^2.

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α - Regularization of QPLS2

A parameter α is introduced to balance the linear and the quadratic terms, $0 \leq \alpha \leq 1$:

$$\alpha \operatorname{cov}^2(u_h, t_h) + (1-\alpha)\operatorname{cov}^2(u_h, t_h^2)$$

α is set to the value that leads to the highest R_Y^2 coefficient of the quadratic model.

During the deflation step, Y is deflated using t and t^2.

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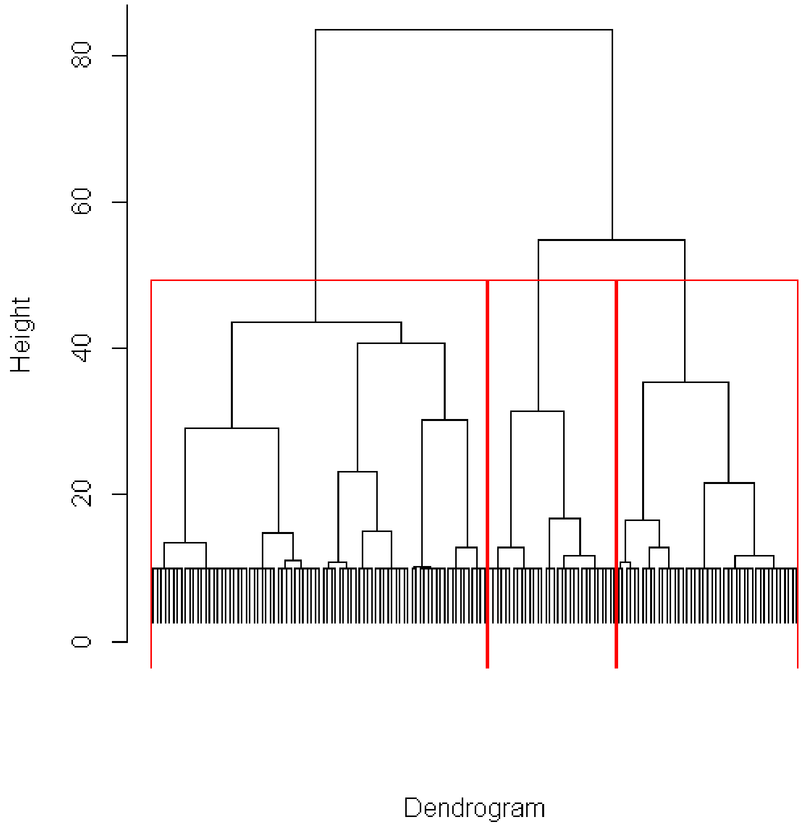
Application to Preference Mapping : The Coffee dataset (ESN, 1996)

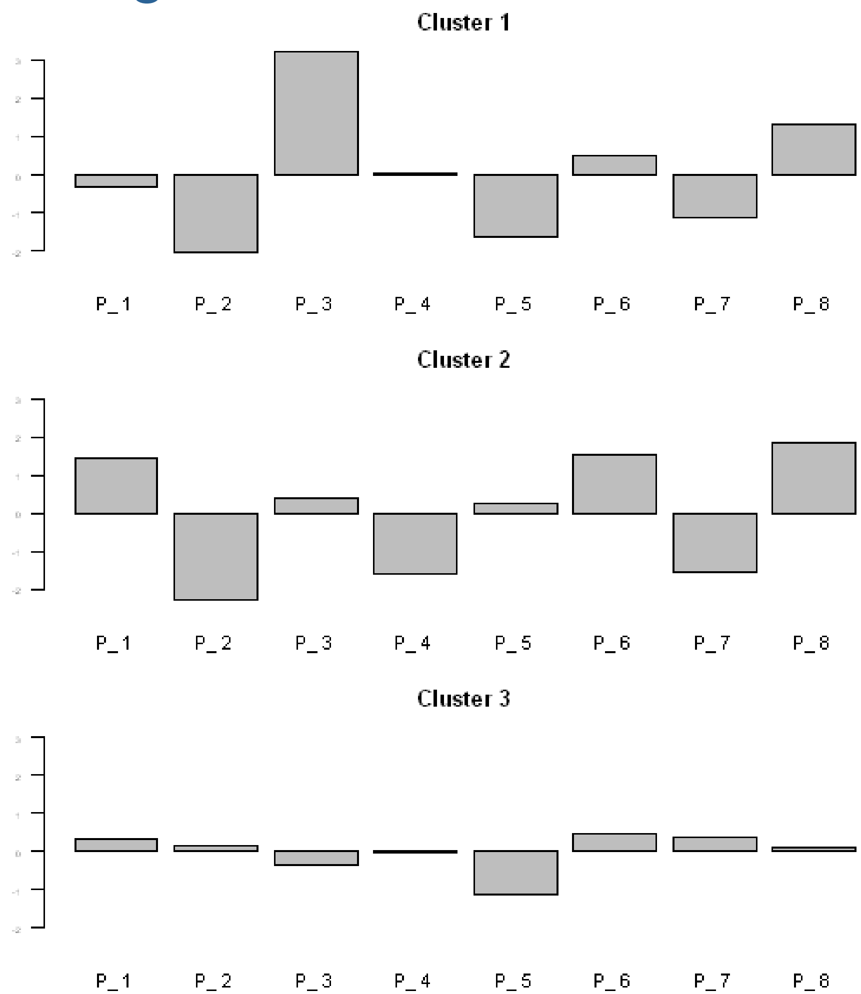
Data

- 8 coffees
- 160 french consumers who have been partitionned in 3 clusters
- Quantitative descriptive analysis: 23 sensory descriptors
    - Smell descriptors : chocolate, intensity, moisty, sweet...
    - Taste descriptors : sour, chocolate, metallic...

Application to Preference Mapping : The Coffee dataset

Results of the Hierarchical Clustering:

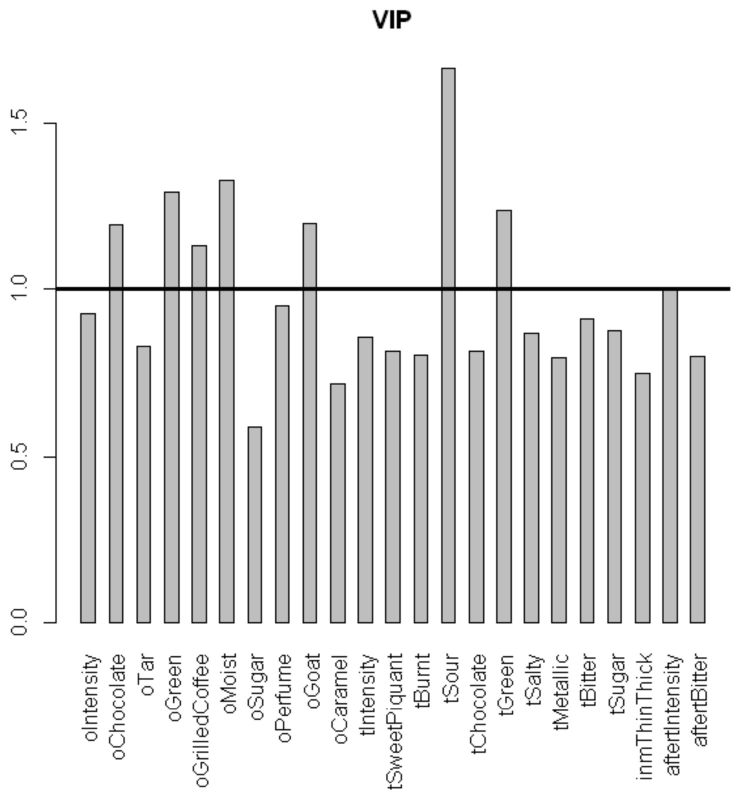


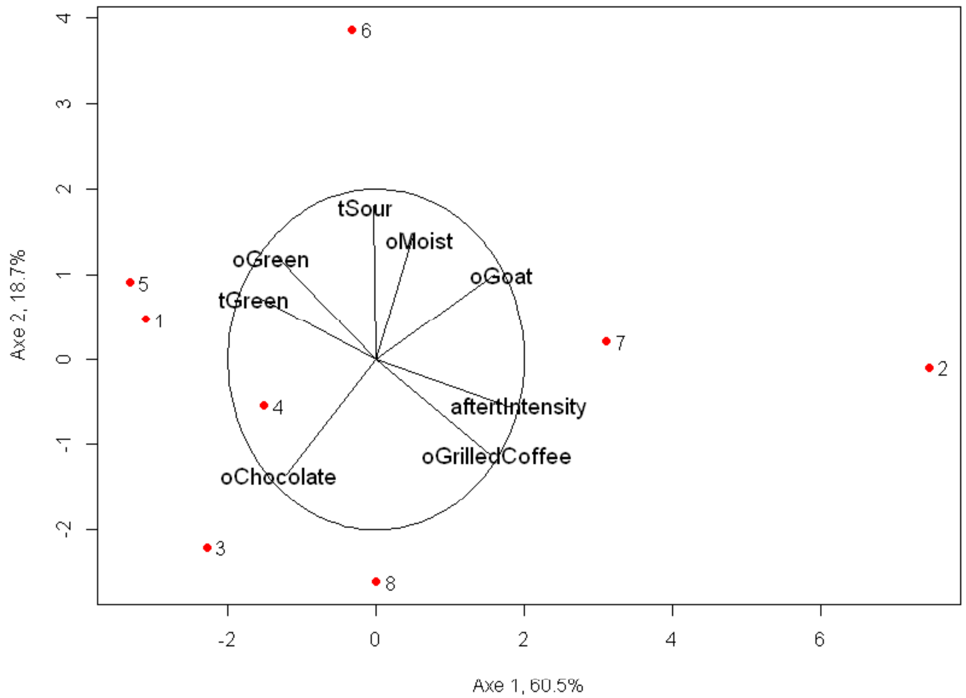


Application to Preference Mapping : The Coffee dataset

Products map obtained by QPLS:

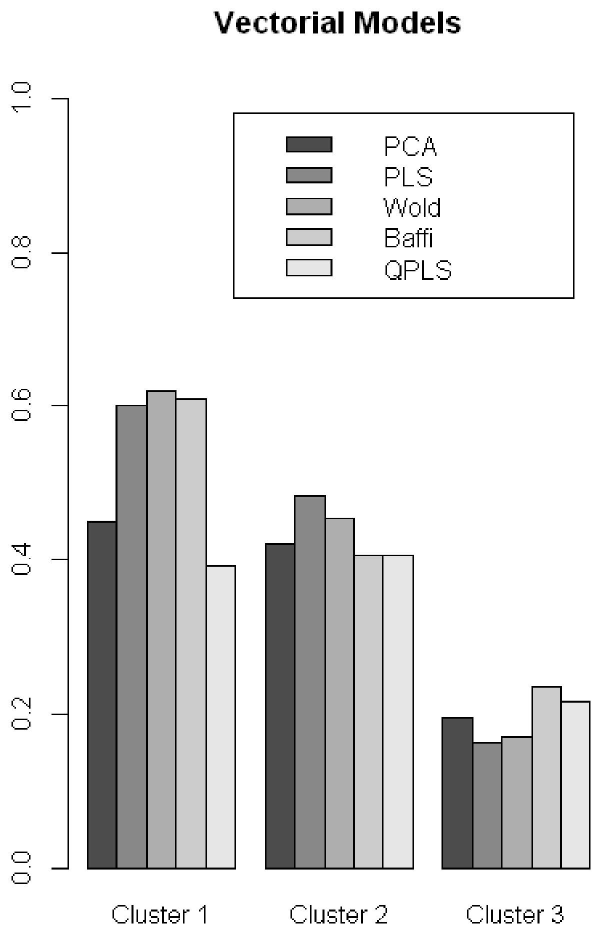
- **~ 79% of the variance of X explained by t_1 and t_2**
- **~ 80% of the variance of Y explained by the quadratic model (t_1, t_2)**

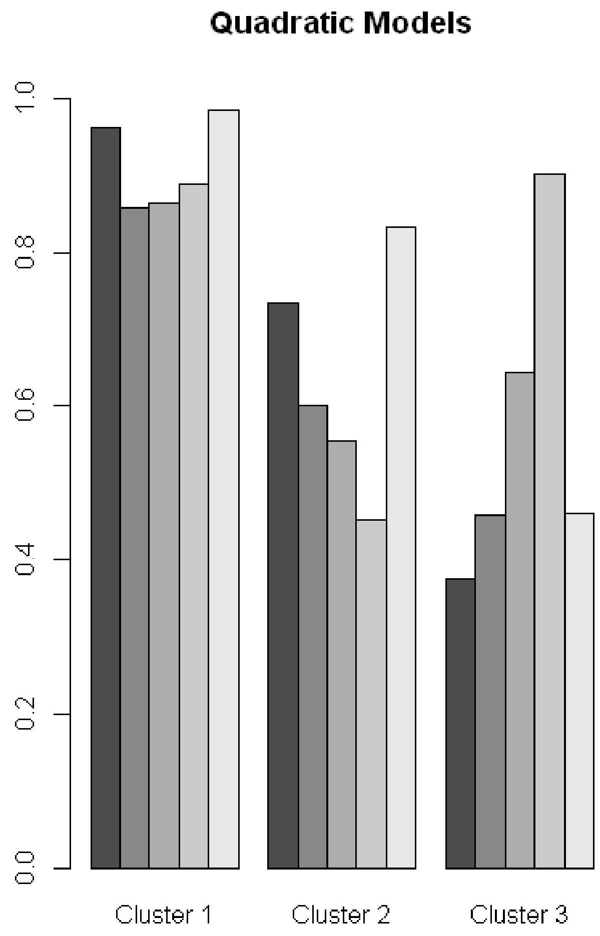




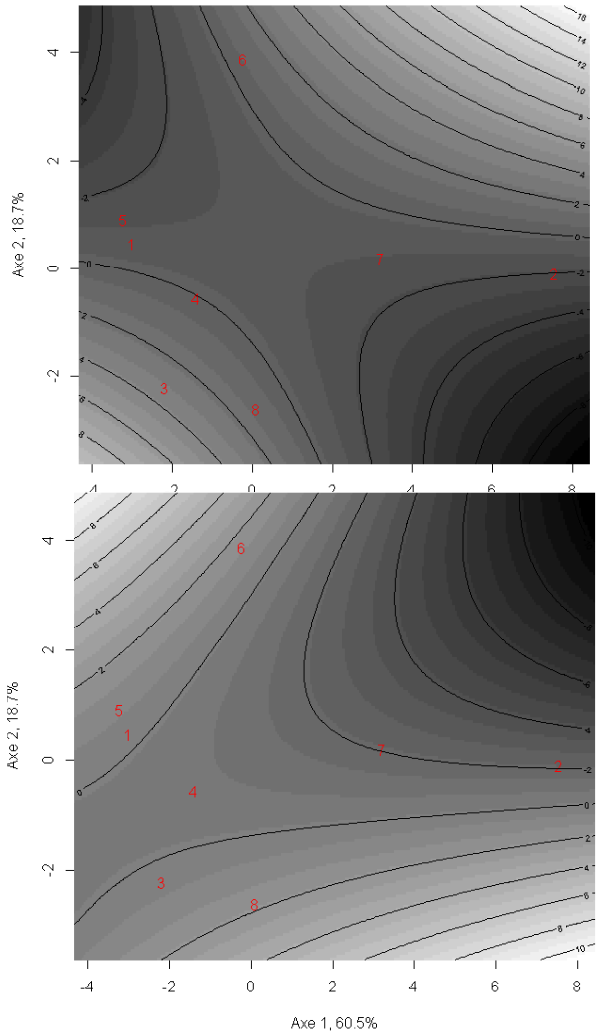
Application to Preference Mapping : The Coffee dataset

R_Y^2 explained for the three clusters





Application to Preference Mapping : The Coffee dataset – Clusters



Consumers like both smooth coffee with chocolate odors and strong coffee with intense odor

Consumers like both the green coffee with a lot of perfume and the bitter coffee with an intense aftertaste and an odor of roasted coffee

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Conclusion

QPLS presents several advantages for preference mapping:

- the criterion is very explicit and in line with PLS regression
- the (new) algorithm is simple and convergent.

But :

- in order to enhance the interpretation of the model, there is a need to operate a model selection.

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QPLS, What else ?

Thank you for your attention