Using R for an efficient and standard analysis of Designs of Experiments.

C.Mokdad[1], N.Antille[1], M.Lepage[1], M.Perrot[1], N.Pineau[1] and H.Vlaeminck[1]

1. Nestlé Research Center, Lausanne, Switzerland

Nestlé Research

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Introduction

Design of Experiments (DOE) is a useful strategy to guide R&D specialists through the planning and execution of experiments and helps them to take data-driven decisions. In food processing, one is generally seeking to assess a set of operating parameters in different processes, which takes time and resources. Instead of a trial and error approach, the DOE helps to get insightful results about the global impact of parameters on the final product, maximizing information from a limited number of trials.

Data scientists at Nestlé R&D have applied this methodology for years, and have found that the R environment is particularly suited for the efficient analysis of such DOE. R is a flexible platform, providing high quality outputs, which can also be used in industry to automatize workflows. In the context of DOE analysis, the following one was developed.

"In the context of DOE analysis, a specific workflow was developed to deal with data generated by expert sensory panels. First, a linear mixed model is used on the raw sensory data to allow us to find significant differences between products (using Fisher's Least Significant Difference as a post-hoc test). Then, a model (usually linear) on the mean sensory data enables to assess the relative importance of the factors of the DOE, and to quantify the effect size of each factor on the sensory. In addition, the sensory data can be represented in a 2D space (Principal Components Analysis) that features the sensory space generated by the products coming from the DOE.

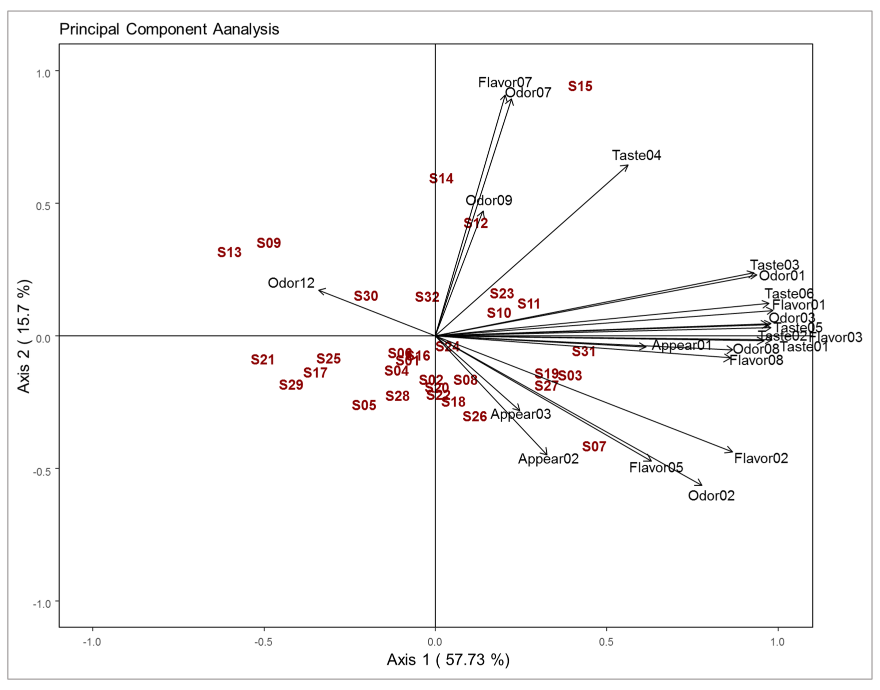
All of these results can be shared with stakeholders using R markdown and/or a Shiny tool, so the final model can be easily used, for instance to predict the sensory profile of any mew product within the studied recipe range.

The example illustrated below is from a 32 samples fractional DOE, built on 13 coffee capsules and extraction factors (type and dosage of coffee in the capsule and 11 machine parameters). A sensory panel of trained people tested all samples to evaluate their sensory characteristics (for example the foam color or the acidity).

1. What is the sensory space generated with the DOE? Are controlled parameters generating significant differences among products?

Sensory space visualization

Principal Components Analysis with FactoMineR's PCA() and ggplot():



Sensory attributes selection

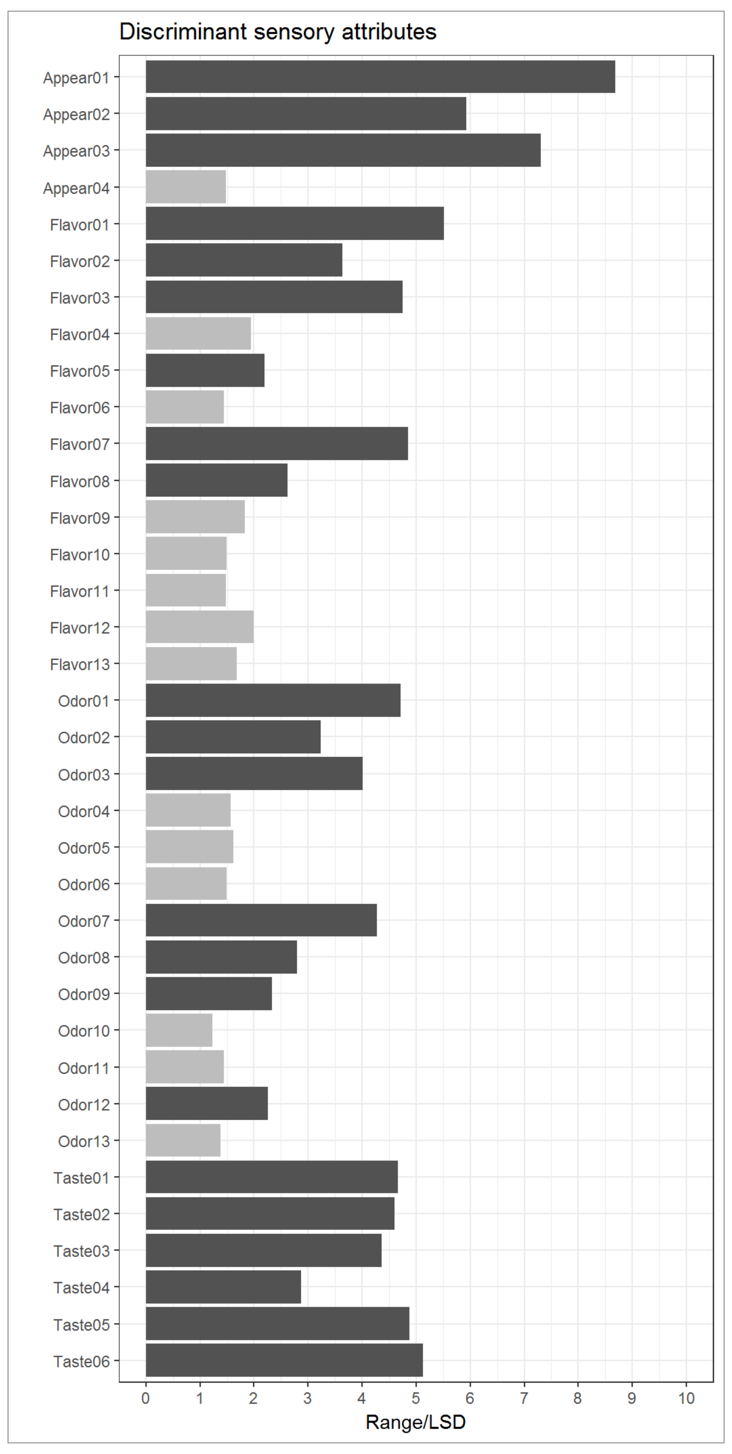
Least Significance Difference (LSD) calculation with lm(), anova() and graphic representation with ggplot():

```
form<-formula("sensory.attribute ~ product + panelist")
mod<-lm(form,temp)
res<-anova(mod)

dl<-res[1][[1]][3]
MSE<-res[3][[1]][3]

LSD<-c(LSD,qt(0.975,df=dl) * sqrt(2*MSE/nb.panelists))
```

+ Range calculated on the samples means



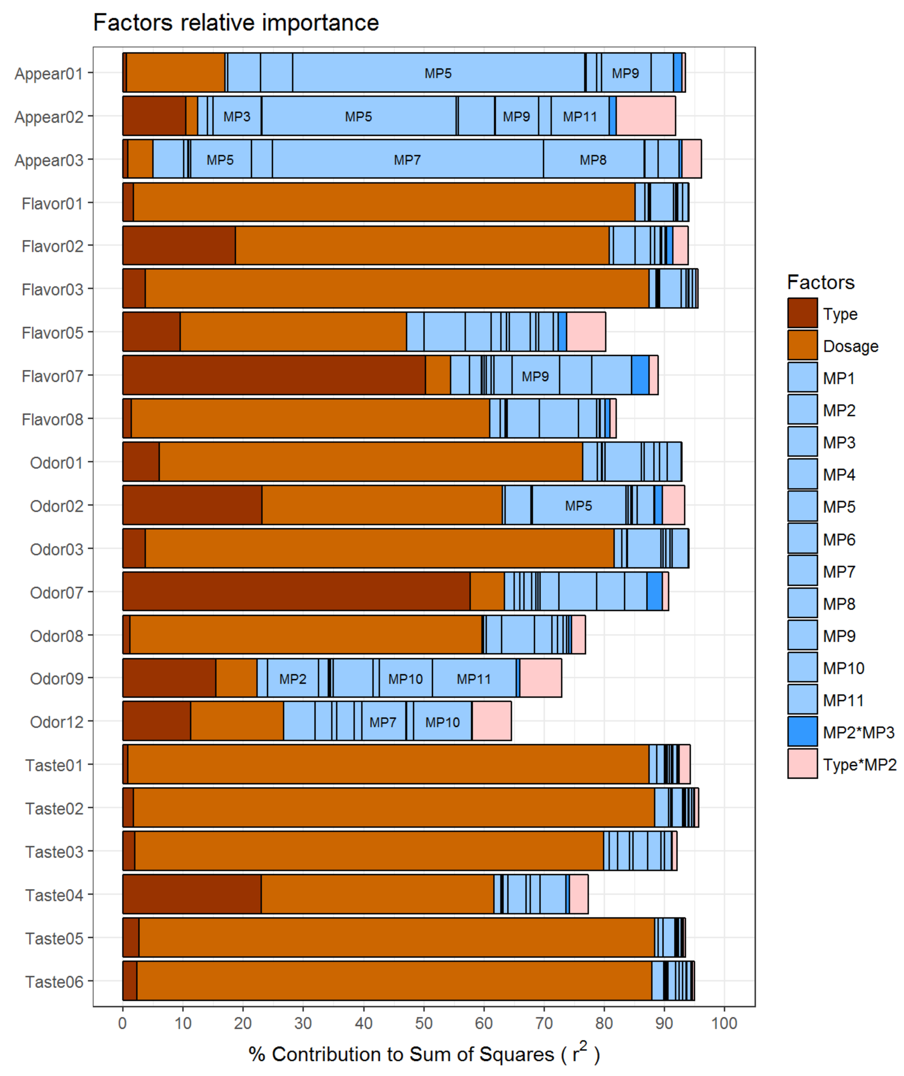
2. Which Machine Parameters have highest relative impact? On what attributes?

```
> form<-formula("senso ~ . + MP2*MP3 + Typ
>   mod<-lm(form,temp)
>   res<-anova(mod)
>   head(res)
Analysis of Variance Table

Response: senso
       Df Sum Sq Mean Sq F value   Pr(>F)
Type    3 0.3227  0.1076  0.2729 0.843582
Dosage  2 9.8675  4.9337 12.5189 0.001894
MP1     2 0.3255  0.1628  0.4130 0.672445
MP2     1 3.2681  3.2681  8.2925 0.016395
MP3     1 3.2402  3.2402  8.2218 0.016744
MP4     1 0.0024  0.0024  0.0060 0.939703
```

Using lm() and anova() and modeling each sensory attribute with the DOE factors, the sum of squares of all parameters and the total sum of squares are extracted. Because samples are from an orthogonal DOE, the contribution of each factor to the total sum of squares is directly calculated as a proportion of the total sum of squares.

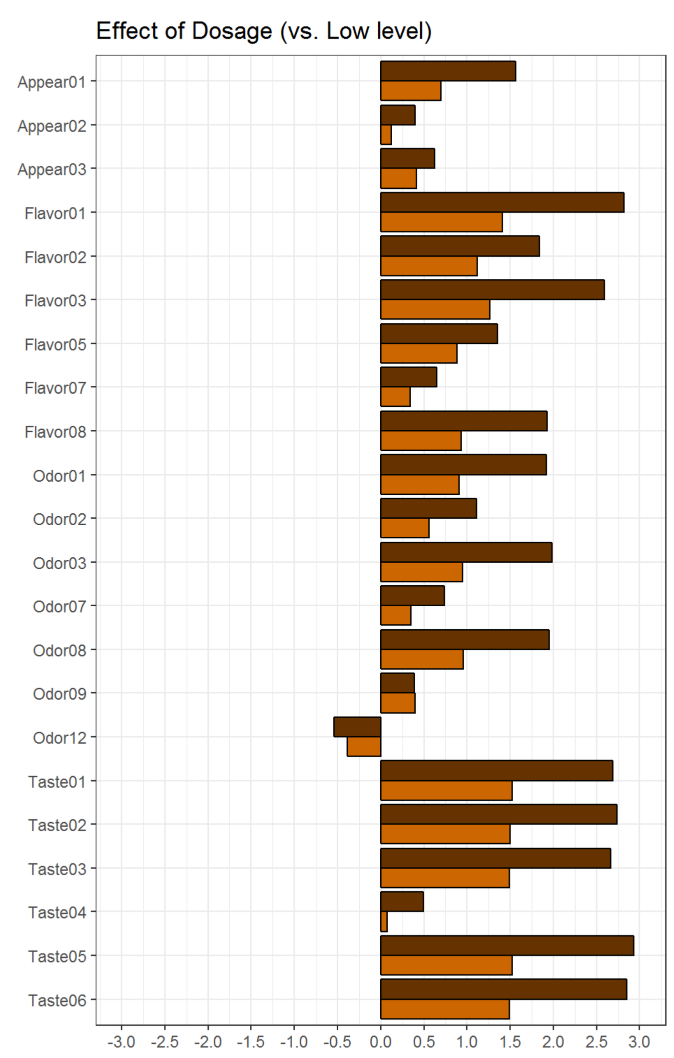
The relative importance for all sensory attributes is plotted with ggplot().

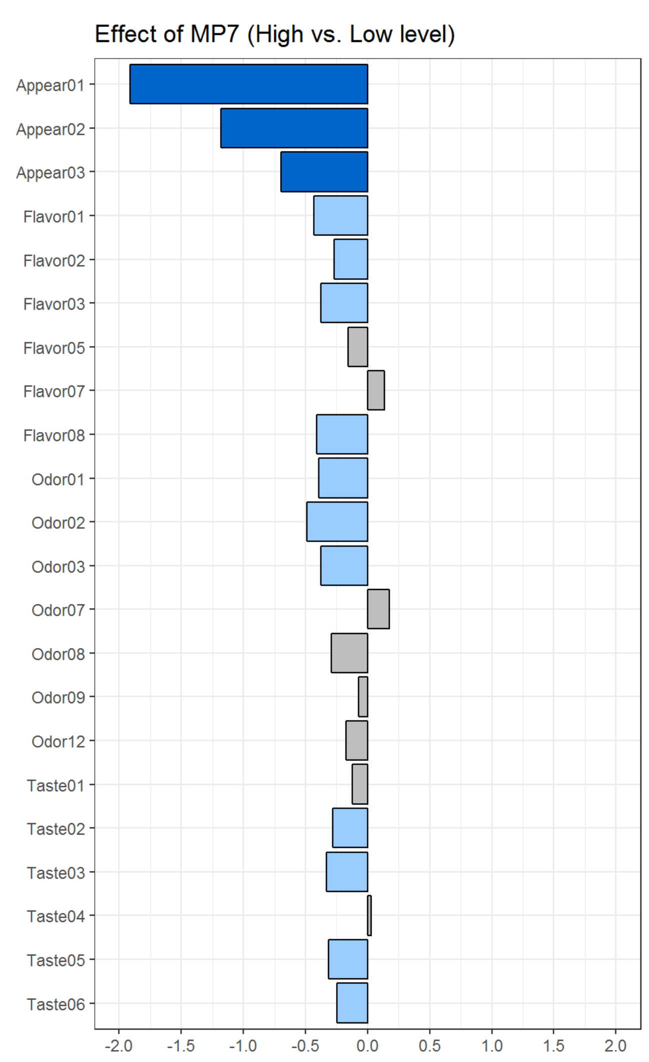


3. What is the absolute impact of each individual parameter on the sensory profile?

Some of the DOE factors like the Dosage were set up with 3 levels, while all Machine Parameters (MP) were set up with two levels. The effect size of each factor is calculated as the average difference between two levels, over all DOE samples. Functions like melt() (reshape package) or summaryBy() (doBy package) are often used to rearrange the data and calculate these effects.

ggplot() is used to plot the effects size. For each factor, the LSD previously calculated is adjusted (divided by the squared root of the number of samples per level) and used as a significance threshold of the effects sizes.





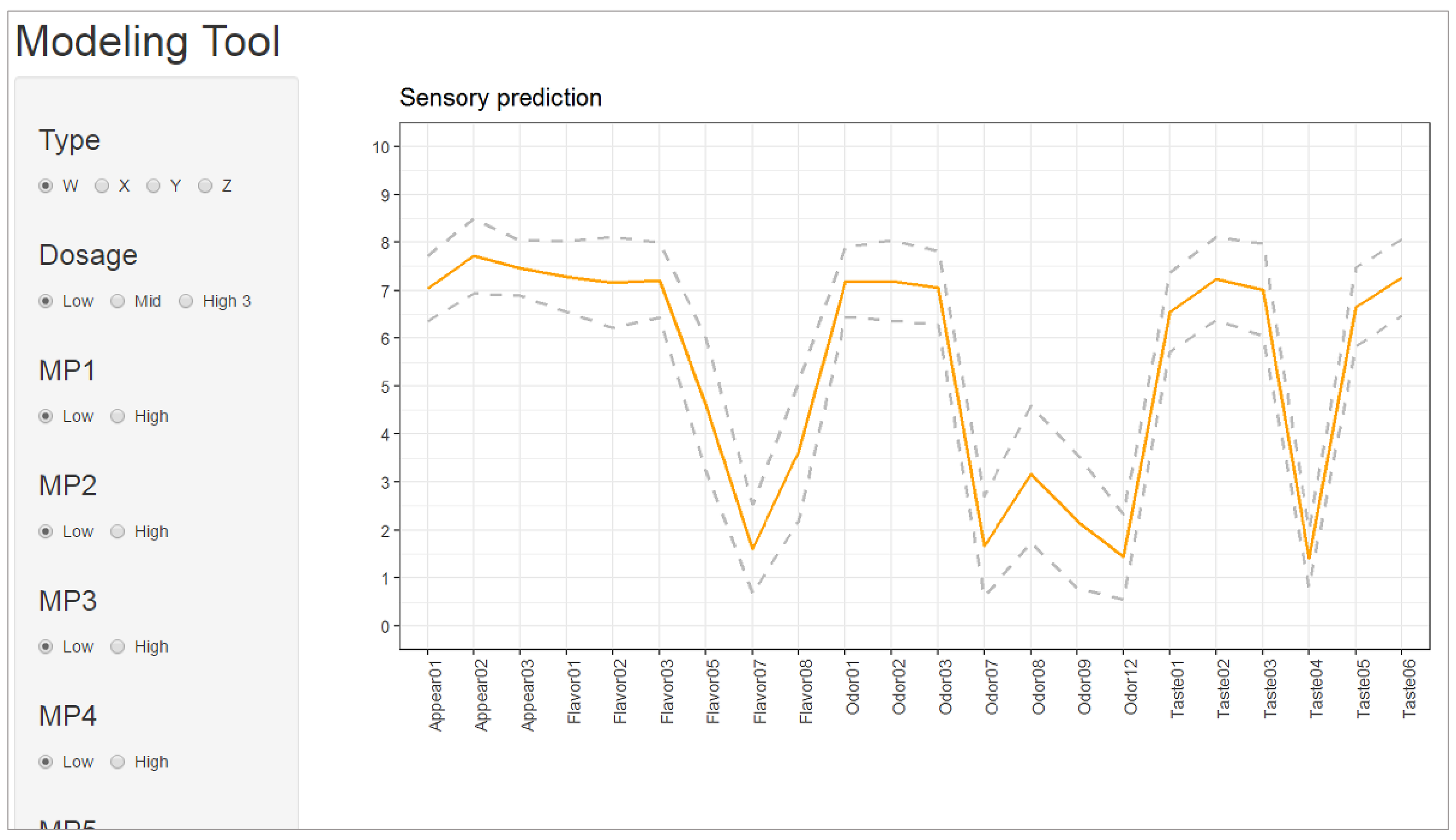
For example, MP7 has an important effect on Appear01 (effect size ≥ LSD) colored in dark blue.

Other effects colored in light blue represent effects to be further investigated (effect size between adjusted LSD and LSD).

All other effects are considered as noise.

4. What parameters settings can produce a specific sensory profile?

Modeling allows to predict a sensory profile with a given combinations of factors' levels. Models are more and more shared with stakeholders through Shiny tools. By selecting any combination of factors' levels, the user can see the sensory prediction, within a +/- LSD interval around this prediction.



Using for example lp() (lpsolve package), an optimization module can also be included to do reverse engineering and find out how to achieve a given sensory profile. By targeting sensory attributes of interest, the tool can suggest a combination of factors levels to reach this target.

Conclusion

R enables to use standard outputs (plots and models) and to efficiently share and reuse this workflow among the data scientists. It also allows to generate reports in a very efficient way using knitr package. Moreover, R also allows to develop Shiny tools which provide a user-friendly interface to stakeholders. An internal shiny tools platform was developed to access these tools and to communicate even further designs of experiments results and outcomes.