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Short Communication

Using fractional factorial designs with mixture constraints to improve nutritional value and sensory properties of processed food

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ABSTRACT

Recipes in cookbooks are presented as a list of directions describing how to cook fixed amounts of ingredients to prepare pleasurable food. Similarly, industrial food products can be considered as processed mixtures of ingredients for which process parameters and mixture parameters should be investigated simultaneously when trying to improve their nutritional and sensorial properties. This work proposes a simple, generic and efficient approach to combine process and mixture factors in the same design by handling easily any mixture constraint in the frame of fractional factorial designs. The approach has been successfully applied in many situations and is illustrated through a case study to improve an all-family cereal recipe both in terms of nutritional value (i.e. 50% sugar reduction and partial replacement of refined wheat flour by whole grains) and sensory properties.

1. Introduction

Industrial food products can be simply described as processed mixtures of ingredients, but the complexity of product innovation and renovation lies in the fact that both process and mixture are highly multifactorial (i.e. often dozens of ingredients processed using multiple complex steps such as drying, roasting, cooking, mixing or homogenizing, each of them being described by multiple factors such as temperature, pressure or duration). In order to cope with this complexity, it is not surprising that the impact on product characteristics of process factors and mixture factors are often investigated separately (using respectively classical factorial design and classical mixture design techniques), although this one-group-of-factor-at-a-time approach suffers the same drawback as the one-factor-at-a-time approach, namely that it leads to local instead of global solutions.

Combining process and mixture factors in the same design is therefore a necessity that various authors discussed in the past. Scheffé (1963) proposed to make all combinations of a mixture design and a factorial design (i.e. Mixture × Process). As an example, Naes, Faergestad, and Cornell (1998) used a design with 10 mixtures and 3^2 process factors (10×3^2) leading to 90 experiments. In practice, such numbers of experiments are much too large for sensory assessments. As a consequence, Cornell (2002) proposed to combine independent fractions of mixture and process but this approach covers the experimental region in a highly non-homogenous way. More recently, approaches such as D-optimal designs (L'Hocine & Pitre, 2016) or space-filling designs (Beal, Claeys-Bruno, & Sergent, 2014) became popular because they are designed to "optimally" cover any type of experimental region, but defining optimality is unfortunately not straight-forward in the food context. On one hand, D-optimality (as well as other common optimality criteria such as A, C, E or I-optimality) is bound to the underlying model (i.e. D-optimality minimizes the overall variance of the estimated regression coefficients), but this underlying model is generally unknown, especially for highly multivariate responses such as sensory profiles. On the other hand, coverage optimality is completely independent of any model but is bound to the definition of a distance between any two points of the experimental region (i.e. it minimizes the maximal distance between any point of the experimental region with its nearest experiment), and defining accurately such a distance is still an unsolved problem in case of highly asymmetrical experimental regions (which is common when mixing macro-nutrients, with ranges typically smaller than 10%, and micro-nutrients, with ranges typically smaller than 1%).

In order to overcome these issues, we propose an easy procedure for incorporating common mixture constraints into classical fractional factorial designs. This very flexible approach has been

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presented at Agrostat symposium in Lausanne (Rytz et al., 2016) and is illustrated here through an example on all-family cereals. Schematically, a basic all-family cereal recipe is made of 80% wheat flour and 20% sucrose that is mixed, soaked, cooked and dried. In order to improve the nutritional value of the product, the aim was to reduce its final sugar content by 50%, without using any intense sweetener or flavour, while maintaining or improving sensory properties. Since a simple recipe with 90% wheat flour and 10% sucrose is rejected by consumers, a two-step approach consisting of the following steps was used:

1) A design with 8 experiments to test whether natural generation of biscuit and caramel notes during the process could be a winning strategy thanks to their congruency with perceived sweetness (as previously demonstrated for model systems by Labbe, Rytz, Morgenegg, Ali, and Martin (2007)).
2) A design with 16 experiments to optimise nutritional offer by replacing part of the wheat flour by whole grain.

These two steps led to a final product composition of 75% wheat starch, 15% whole grains and 10% total sugars.

2. Material and method

2.1. Mixture designs to handle mixture constraint

Most food products are mixtures of q ingredients. Each ingredient can vary in quantity x_i ($i = 1\ldots q$) but they have to sum to a constant c. The basic constraints of an experiment with mixtures are:

$$\sum_{i=1}^{q} x_i = c \text{ and } 0 \leqslant x_i \leqslant c, \; i = 1, 2, \ldots, q$$

In this simple case, the experimental region is a simplex that Scheffé (1958) proposed to cover homogeneously with simplex-lattice and simplex-centroid designs. In most food experiments, additional constraints have to be introduced, namely that most ingredients have to vary in ranges that are bound by lower (a_i) and upper (b_i) limits:

$$0 \leqslant a_i \leqslant x_i \leqslant b_i \leqslant c (i = 1 \cdots q)$$

In this more general case, the experimental region is no more a simplex, but a hyper-polyhedron. Cornell (2002) made an excellent review of different approaches to cover such hyper-polyhedron, including extreme vertices designs (with associated XVERT algorithm basing on an A-optimality criterion), Saxena and Nigam designs, D-optimal designs or space-filling designs. A nice example of such an experimental design that optimised sensory properties of pizza while reducing salt is given by Guilloux, Prost, Courcoux, Le Bail, and Lethuaut (2015).

2.2. Box-Hau projected fractional factorial designs to handle mixture constraint

Box and Hau (2001) proposed a procedure that allows fractionating simultaneously the mixture and the process parts. For a food product consisting of q ingredients to be processed according to n factors, the basic idea is to build a full factorial 2^{q+n} or a fractional factorial 2^{q+n-a} (Box, Hunter, & Hunter, 2005) or any orthogonal array (Hedayat, Sloane, & Stuken, 1999) and then to project this initial design onto the hyper-polyhedron defined by the mixture restrictions. As an example, Bjerke, Naes, and Ellekjaer (1999) use a 2^{5-1} fractional factorial design including two 2-levels process factors and three projected mixture factors. Other examples allow handling double mixtures (Dingstad, Egelandsdal, & Naes, 2003) or split-plot structures (Måge & Naes, 2005). The flexibility and efficiency that Hau and Box introduced with their projection is very important in case of near-to-spherical experimental regions, but fails to cover the whole experimental region when dealing with asymmetrical experimental regions, because it relies on a symmetrical arrangement of experiments around a reference.

2.3. Adjusting fractional factorial designs to handle mixture constraint

It is proposed to make profit from all advantages of the Box-Hau projection, while simplifying the adjustment (i.e. no need for a reference point) and making it therefore very generally applicable (i.e. homogeneous covering of asymmetrical experimental regions). The proposed adjustment is described below in three steps.

2.3.1. Step 1: define experimental region

Consider the bounds of the q ingredients as given by the practitioner. Let a_i and b_i respectively be these lower and upper bounds of the ingredients ($i = 1\ldots q$). It is easy to demonstrate that the experimental region is in fact restricted to the following bounds:

$$a'_i = \max\left(a_i;\; c - \sum_{j \neq i} b_j\right)$$

$$b'_i = \min\left(b_i;\; c - \sum_{j \neq i} a_j\right)$$

Only these bounds are further considered.

2.3.2. Step 2: build a pseudo-mixture design based on an orthogonal array

Start with any 2-level orthogonal array D_{Init} consisting in n experiments (e.g. fractional factorial design). For each experiment and each factor, replace the low level by the lower bound a'_i and the high level by the upper bound b'_i. Let us call this new design $D_{Intermediate}$ and its elements x_{ti} ($t = 1\ldots n$, $i = 1\ldots q$). In $D_{Intermediate}$, none or almost none of the mixtures sum to the constant total amount c.

2.3.3. Step 3: transform the pseudo-mixture design into a mixture design

The transformation consists in adjusting the mixtures according to their lack (i.e. $c - \sum x_{tj} > 0$) or excess (i.e. $\sum x_{tj} - c > 0$) of total amount proportionally to the range of variation of their respective components ($b'_i - a'_i$). The final design D_{Final} is defined as follows by its elements x'_{ti} ($t = 1\ldots n$, $i = 1\ldots q$):

$$x'_{ti} = \begin{cases} a'_i + \max\left(0;\; c - \sum_{j=1}^{q} x_{tj}\right) \dfrac{(b'_i - a'_i)}{\sum_{j; x_{tj} = a'_j} (b'_j - a'_j)} & \text{if } x_{ti} = a'_i \\ b'_i - \max\left(0;\; \sum_{j=1}^{q} x_{tj} - c\right) \dfrac{(b'_i - a'_i)}{\sum_{j; x_{tj} = b'_j} (b'_j - a'_j)} & \text{if } x_{ti} = b'_i \end{cases}$$

As an example, let us consider the simple mixture of 3 ingredients with bounds $a_i = a'_i = 0$ and $b_i = b'_i = 1$ ($i = 1, 2, 3$), summing to a constant $c = 1$. Fig. 1 shows that the full factorial design 2^3 generates a simplex-lattice design {3;2} (i.e. simplex with 3 vertices allowing to fit a 2nd order model) with 2 added centre points. In this simple case, the performed adjustment is a central projection (with centre = 0) from the 8 experiments of the 3-dimensional cubus onto the 2-dimensional simplex defined by the vertices A, B and C. Similarly, the fractional factorial design 2^{3-1} defined by experiments P1, P2, P3 and P4 generates a simplex-lattice design {3;1} with 1 added centre point.

The R software (R Development Core Team, 2008) was used to perform all calculations and statistical analyses.