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AUTOMATED FORMULATION OF A BEVERAGE BASED ON THE OPTIMIZATION OF SENSORY PROPERTIES

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ABSTRACT

The formulation of a beverage prepared from a mixture of liquid products was optimized, based on sensory properties, using the simplex algorithm. This method offers many advantages compared to classical methods of optimization such as multiple regression. Because the composition of the sample being tasted depends on the responses to prior samples, on-line preparation of the samples is required. This was achieved through the use of an automated apparatus (AAST) for sample preparation and of a computer for response-processing, feedback to the AAST and judge instruction. Applications of the method include matching a standard product or developing an ideal product.

Keywords: Formulation; sensory analysis; optimization; simplex; automation.

INTRODUCTION

A food product is generally manufactured from a mixture of raw materials. The characteristics of the product (sensory and nutritional properties, safety, price, etc. . . .) depend on a number of variables, including the kinds and sources of raw materials, the proportions of the various ingredients in the product formula and processing variables.

The goal of the food scientist is to formulate the best possible product with the ingredients and processes at hand, that is, to optimize one or several characteristics of the product as a function of various goals and constraints related to the variables listed above.

The purpose of the present article is to present a new method for the formulation of food products based on the search for an optimum. In this method we apply a modified version of the simplex algorithm to sensory formulation. A step-by-step search for the optimum is performed, which requires the use of an automated system. Such a procedure allows one to determine formulations and prepare samples that get closer and closer to an optimum based on an individual's responses to previous samples.

Optimization methods

There have been many studies of product optimization methods for the food industry. Bender *et al.* (1982) used linear programming for the formulation of a low-cost mayonnaise. Lund (1982) optimized product quality based on processing parameters.

Optimization based on the sensory properties of a product traditionally has been achieved with indirect methods (Schutz *et al.*, 1972; Stubblefield & Hale, 1977; Huor *et al.*, 1980; Shen *et al.*, 1980; Henika, 1982; Giovanni, 1983; Bardot *et al.*, 1992). The parameters of the model are adjusted through an experimental design which minimizes the number of sensory assessments. Samples are prepared in advance. The main problem associated with these methods is the dependence of the results on the model chosen in advance. This can be limiting in the case of aromas, the mixture of which is hard to predict with any model (Laing *et al.*, 1989). Also, these methods do not account for biases or errors that the judge may commit during tasting sessions. For these reasons, we opted for a direct optimization method.

Direct optimization methods were introduced by Box (1957). Many algorithms are now available, most of which proceed variable by variable (Rosenbrock, 1960; Hooke & Jeeves, 1961). These *evolutionary operation* methods use factorial designs combined with regression techniques to estimate the direction of steepest ascent and to locate the optimum region of a response surface (Morgan & Deming, 1974). The selection of the proper algorithm for sensory tests is crucial because, in sensory evaluation, the number of trials or assessments quickly becomes limiting. It is therefore imperative to use a method which quickly converges towards the optimum. We selected the modified simplex method proposed by Nelder and Mead (1965). This sequential method is a highly efficient, multifactor, empirical feedback strategy that requires neither the large number of trials nor the complex calculations of the *evolutionary operation* methods.

It optimizes the step size of the simplex at each step and reaches the optimum by convergence in less than twenty trials (Morgan & Deming, 1974). The simplex algorithm has been successfully used to optimize reactional mixtures in chemistry (Porte *et al.*, 1984; Phan-Tan-Lu *et al.*, 1979) and beverages (Williams, 1989*a*,*b*).

The main drawback of direct optimization methods is that, unlike commonly used indirect methods, they require on-line preparation of the samples because the formulation of the sample presented to the judge depends on prior sample's evaluations. The test protocol was modified to meet this requirement: preparation of the samples was automated and judge instruction, data collection and statistical analysis where computerized. The automation of sensory measurements also eliminates many experimental biases (Hossenlopp *et al.*, 1989).

The purpose of this study was to apply the simplex method to match a reference by minimizing the sensory difference between the samples and the reference in a stepwise fashion. In this study, we focused on the sensory properties of the product in the optimization process. The results from this experiment, where a *known* reference was copied, will aid in the development of further studies in which the method would be used to copy an existing food product (Méhu, 1989) or to formulate a product based on hedonics (*ad libitum* formulation).

MATERIALS AND METHODS

Products

The purpose of the experiment was to copy a known reference containing 3% v/v strawberry syrup and 2% v/v apple syrup in water. The quality of the match obtained by the judge was then assessed by comparing its composition to that of the reference. The samples to be compared to the reference were prepared by an automated apparatus (Fig. 1) which mixed (1) 20% v/v strawberry syrup, (2) 20% v/v apple syrup and (3) mineral water (Volvic^{TM}) in proportions determined by a calculation module.

Judges

The panel consisted of seventeen judges (7 male and 10 female), between 17 and 48 years of age, all of them students or university staff.

Sensory attribute

The judge was asked to scale the overall sensory difference between each sample and the reference. That difference was the function being minimized through

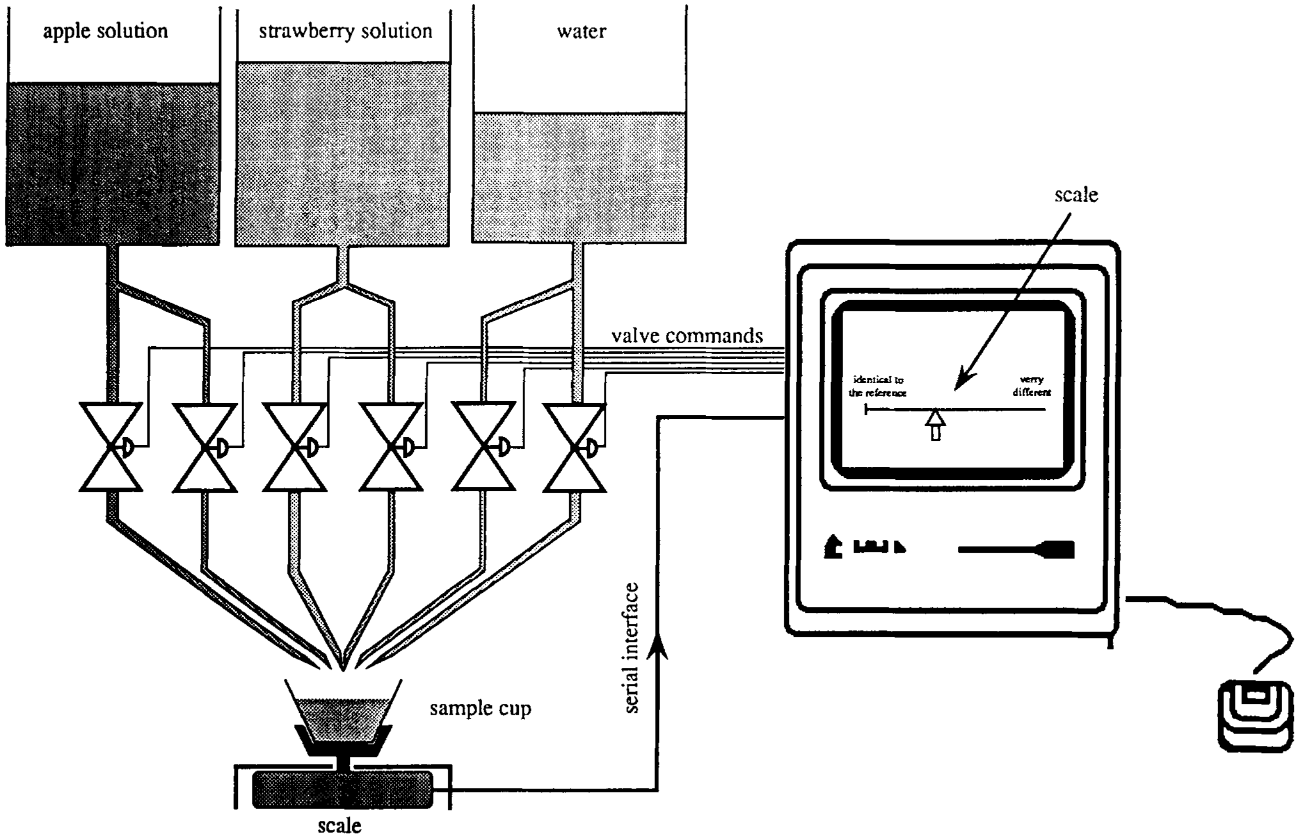


FIG. 1. Operating principles of the automated apparatus for sensory testing (AAST).

the simplex procedure. The scaling of the difference between a sample and a reference is based on the same principle as similarity ratings which compare samples two by two. It should be emphasized that the sensory space in which the samples and the reference may be characterized is a multidimensional continuum. In a sensory measurement, the judge evaluates the difference between samples and the reference along several dimensions. That is in contrast with physical measurements which monitor differences along one dimension. An unstructured graphic scale, anchored with the terms *identical to the reference* and *very different*, was used to scale the difference (Schiffman *et al.*, 1981). This scale is suited for computerized data collection (Barthélemy *et al.*, 1990). Using a mouse, the judge marked the scale displayed on the monitor to indicate the intensity of the difference. An interlaboratory study (Lungred *et al.*, 1986) demonstrated the validity and reproducibility of this type of scale across a variety of sensory tests.

Optimization algorithm

The modified simplex designed by Nelder and Mead (1965) was used. The function to minimize was the judge's difference rating between samples and the reference, a function of 2 variables—the proportion of strawberry (1) and apple (2) solutions.

Initial simplex

The following three samples made up the initial simplex for all judges (Figs 2 and 3):

sample 1	6% strawberry solution	6% apple solution
sample 2	6% strawberry solution	8% apple solution
sample 3	8% strawberry solution	6% apple solution

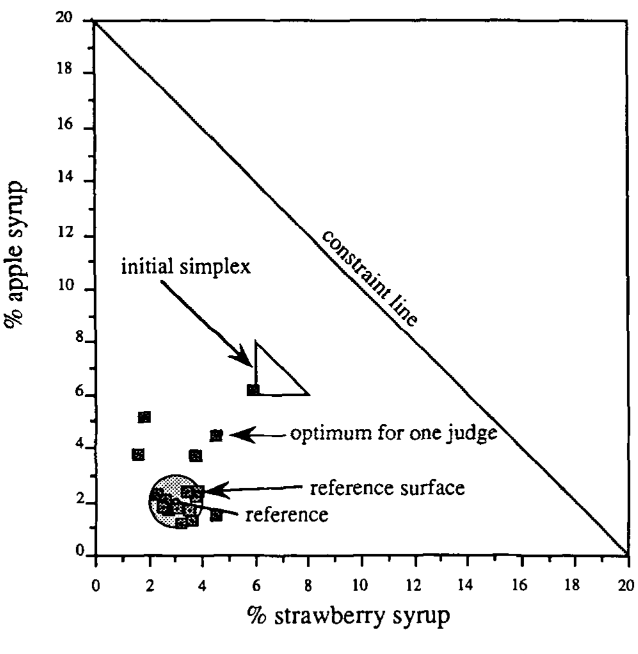
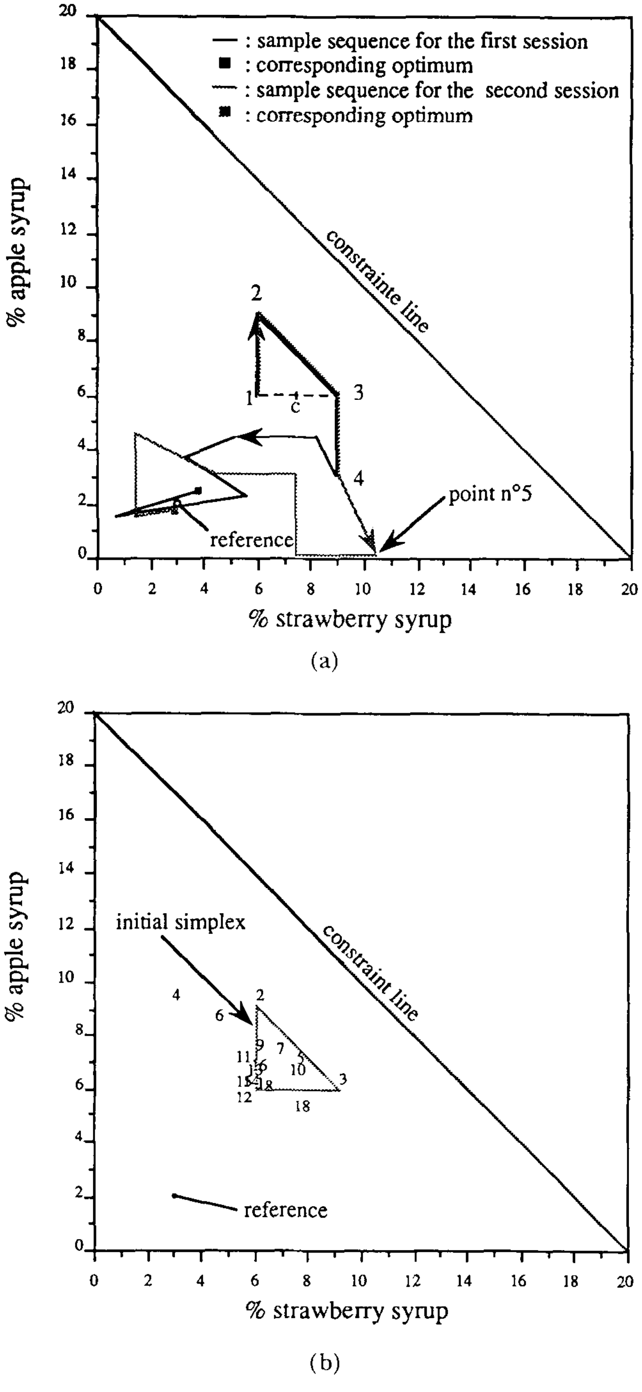


FIG. 2. Location of the optima produced by the 17 judges.



(a)

(b)

FIG. 3. (a) Illustration of the progression of a judge towards the reference during two consecutive sessions. (b) Example of premature convergence.

Principle of the algorithm

The principle of the simplex method (Spendley *et al.*, 1962) and of the modified simplex method is to eliminate the worst of the three samples evaluated by the judge (i.e. the one with the highest difference rating) and to replace it with a sample closer to the optimum. This principle is illustrated in Fig. 3a. The simplex is a geometric figure defined by three points, that is, one more than the number of dimensions of the variable space (2). In the initial simplex, sample 3 gave the best response (smallest difference rating), sample 2 gave the worst response and sample 1 gave the next-to-worst response. C is the centroid of the face remaining when the worst sample is eliminated. The composition of the new sample is defined by extending the line segment between sample 2 and C by a factor of two beyond C to generate sample 4. The same process is repeated with the three new samples. This method allows for the expansion or the contraction of the simplex to adjust its size according to the phase of the optimization process (i.e. quick, rough search of the optimum at first, followed by a finer search). The respective values of the expansion and contraction coefficients were 2 and 0·5. The 'best' formulation obtained by this method was then presented to the judge and the program iterated in the same way until an optimum was found, that is to say until the stopping criterion was reached.

Stopping criterion

Determining a stopping criterion proved to be difficult. In this particular sensory test (matching a reference), it was possible to interrupt the tasting session when the perceived difference between the sample and the reference was small. We elected to stop the session when the average of the difference ratings of the last simplex was below 10 on the 0–100 scale. At this point, it was considered that the variation brought about by a new point was not significant anymore.

To take into account judge fatigue, the maximum number of trials per session was set at twenty. This number is high enough to allow convergence in most cases (Morgan & Deming, 1974), and it accommodates sensory constraints.

Constraints

The search for the optimum is limited by physical constraints, such as the impossibility of serving negative volumes or technological ones, such as the smallest possible volume that can be accurately measured. Economical considerations set by the experimenter may also be constraints. In this experiment, we introduced the following physical constraints only:

$$Vs > 0,\ Va < 0 \text{ and } Vs + Va < 20 \text{ ml (sample volume)},$$

where Vs is the volume of strawberry solution and Va the volume of apple solution.

Any mixture which fell outside the above constraints (beyond the constraint line) was not presented to the judge and was assigned a high arbitrary difference rating which made it the worst sample in the simplex being evaluated.

Validation of the optimum

Validation is an essential part of the experiment. In the case of an imitation test, the optimum formula is obtained when there is no detectable difference between the sample and the reference. The optimum formulations were validated by having the judges perform triangle tests between the sample and the reference. These triangle tests were automated using the same apparatus as for the simplex procedure (Hossenlopp *et al.*, 1989) and analyzed with Wald's sequential test (1947).

The automated apparatus for sensory testing

The composition of a sample depends on the difference rating given by the judge to prior samples. The required on-line preparation of the samples cannot be achieved manually. An automated apparatus for sensory testing (AAST) was designed to carry out the following functions: (1) preparation of the samples, (2) dialogue with the judge and (3) processing of the judge's responses (especially the sequential calculation of the composition of the next sample). This automated apparatus (Fig. 1) is a modified version of the apparatus described by Heyd *et al.* (1989). The microcomputer used in connection with the AAST was a Macintosh® SE.

Sample preparation

The AAST allows for the automatic delivery to the judge of samples varying in the proportions of strawberry and apple solutions. These samples were prepared by mixing the solutions and the water in proportions determined by the microcomputer. The samples were presented at room temperature (20°C).

Each solution to be mixed into the sample cup flows by gravity. The flow is controlled by two clamp-valves interfaced with the microcomputer through an analog to digital converter. The apparatus has two networks of feed lines. The first one, with a flow rate of 2·5 ml/s, is used to approach quickly the programmed volume, and the second one, with a flow rate of 0·5 ml/s, is used to accurately and precisely reach it.

The weights of solutions delivered by the apparatus are controlled with a precision scale (1 mg) interfaced to the microcomputer. The software converts weights into volumes and commands the opening or closing of the valves accordingly.

Dialogue with the judge

The apparatus was used in a self-service fashion by the judge. The program identified the judge and gave him/her instructions on the monitor. The judge did not know the composition of the samples being served.

The judge went through the following sequence of events: (1) place the empty cup on the scale, (2) rinse his/her mouth with water while the next sample is being prepared, (3) taste the new sample, (4) compare it to the reference and (5) mark his/her response on the scale.

When the program determined that the session was over (i.e. the maximum number of trials has been reached or the algorithm has converged to the optimum), the judge was dismissed. A session took about 30 min.

Data processing

The computer program processed the responses of the judge at each step according to the simplex algorithm, determined the composition of the next sample and commanded its preparation. The responses were also saved in a file.

RESULTS AND DISCUSSION

Performance of the apparatus

The apparatus afforded good precision in the preparation of the samples. The standard deviation for the sample volume was 0·02 ml. This value is well below the difference threshold (for visual perception of differences in sample volume) of 1 ml measured for the panel.

The average mixing time was below 20 s for 20-ml samples. This time is not too long because it allows the judge to rinse between samples and to get ready for the next trial.

During the experiments, there was no reliability problem with the equipment. The use of sweetened products did not cause any plugging of the tubing, nor did it affect the performance of the apparatus. A daily cleaning of the apparatus was required. The accuracy of the measured volumes was maintained. There was no interference between the aromatic compounds in the solutions because the two circuits are completely separate and the tasting cups are used only once and disposed of thereafter. The use of clamp-valves allows for easy replacement of the tubing. This is particularly important to avoid contamination among products when different products are being tested.

Formulation results

The triangle tests conducted to compare the optimum and the reference showed that there was no significant difference between the two when the optimum was inside a circle called the *reference surface*, centered at the point corresponding to the composition of the reference, with a radius of 1 (Fig. 2). Any optimum located inside the *reference surface* cannot be improved. On the other hand, judges whose optimum is located outside of the *reference surface* can detect the difference with the reference in the triangle test, and their responses subsequently can be eliminated.

Figure 2 shows that 11 out of 17 judges produced an optimum located inside the *reference surface.* Considering the difficulty of the task—high amount of sugar in the samples, complexity of the strawberry and apple aromas—the method proved to be efficient by reaching the optimum formula in 65% of the cases over a short period of time (less than 30 min).

Figure 3a shows the progression of a judge towards the reference in two sessions conducted on two consecutive days. The judge converged to the optimum in 10 trials during the first session, and in 11 trials during the second one. Convergence was achieved in both sessions, although different paths were used by the judge. It is concluded that the method is reproducible. It is also worth noting that the simplex method affords some correction of judge error in the evaluation process (Porte *et al.*, 1984). For example, Figure 3a shows that in the second session, the algorithm proposed sample 5, which actually is a step away from the reference. This point was rejected as the worst of the three points in the new simplex, and optimization then proceeded in the right direction.

Six judges, however, did not reach the reference surface (Fig. 2). In each case this was due to premature contractions of the simplex during the progression. One example is shown in Fig. 3b. The first three samples making up the three points of the initial simplex are clearly visible, but a contraction of the simplex led to the drawing together of the samples. Contractions usually take place near the optimum in order to refine its determination. However, when a contraction happens due to judge error early on in the optimization process, it does so in a zone away from the optimum. In turn, the difference among samples becomes smaller, whereas the difference between the samples and the reference gets larger. Scaling the difference becomes more difficult for the judge (Fishken, 1983), which in turn increases the chances for judge error and simplex contraction. When the judge cannot converge properly, the triangle test establishes that he/she can detect the difference between the optimum towards which he/she is converging and the reference.

Premature contraction is a drawback of the modified simplex method when it is used to monitor a response with a high level of noise or background (Routh *et al.*, 1977). Such is often the case with a sensory response. This drawback could be eliminated by using the super modified simplex method presented by Routh *et al.* (1977).

According to these results, the proposed method has proved both efficient and appropriate for sensory formulation. The same kind of approach could be used for hedonic applications (Heyd, 1991). Although some formulations (35% of cases) did not lead to any conclusive result, the coupling of this testing method with validation tests should guarantee the validity of the optimum reached.

CONCLUSIONS

This study demonstrated the potential of the automation of the formulation of food products based on sensory properties. The use of the AAST simplified the test protocol and reduced the biases normally associated with sensory experiments. This resulted in improved reproducibility of the measurements.

The simplex algorithm proved to be a useful technique for the optimization of a food product formulation in matching an existing product. Indeed, the optimum reached by 65% of the judges was not significantly different from the reference. The simplex method could also be used in the formulation of an 'ideal' product using hedonic ratings. The simplex method requires the instantaneous, on-line preparation of the samples, a requirement which was met with the AAST.

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