Title

Sensory cut-off point obtained from survival analysis statistics

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Abstract

In the present work we applied interval-censored survival analysis techniques to estimate sensory cut-off points based on consumer's decision to accept or reject food products taking into account the inherent variability in sensory measurements. We compared the values obtained using this survival analysis methodology with those obtained by applying a previous regression based method. Cut-off point (COP) estimations were made for acid flavor in yogurt, strawberry flavor in a strawberry flavored drink and appearance quality index in broccoli. For two of these products the regression based cut-off points were unrealistic, and would lead to much too conservative COP's, leading to unnecessary rejection of samples in quality control inspections or very short shelf-lives. For one of the products (strawberry flavored drink), the survival and regression-based COP's were comparable. The survival analysis methodology is recommended for estimating sensory cut-off points in food products.

Keywords: cut-off point, interval-censored data, sensory, survival analysis, shelf life, quality control.

1 Introduction

To illustrate the basics of the cut-off point methodology (Hough, 2010) suppose we are to measure the sensory shelf life (SSL) of sunflower oil. Samples are stored at 45°C for 90 days and every 8 to 10 days a trained sensory panel measures oxidized flavor versus a control sample stored at 4°C. The higher the storage time the higher the oxidized flavor. To be able to establish the SSL some decision has to be taken regarding the maximum level of oxidized flavor that will be tolerated by consumers. If, for example, the maximum level is taken= 2 on the 0 to 10 sensory scale, then the estimated shelf life would be, say, 25 days; if the maximum level is taken= 4 then the estimated shelf life would be 70 days. The key issue is how to establish the maximum level which we shall call the cut-off point (COP).

Hough & Garitta (2012) reviewed the cut-off-point (COP) methodology in estimating sensory shelf life of foods. They categorized this methodology in 'Arbitrary' and 'Regression-based'. An example of an 'Arbitrary' COP was the one used by Villanueva and Trindade (2010) to estimate the SSL of chocolate and carrot cup-cakes. The end of shelf life was determined as the storage time at which the quality limit decreased to the pre-established value of 5.0. In one section of their paper they mentioned that this limit was chosen due to the manufacturer's request, and in another they refer to Gacula (1975). An example of a 'Regression-based' COP was the one used by Garitta et al. (2004) for plastic flavor in dulce de leche. A consumer panel measured acceptability of samples with different levels of plastic flavor. A least significant difference was calculated from this data, and this value was subtracted from the mean liking score for the control sample to provide a minimum acceptable liking score. Next, the consumer data were related to the plastic flavor ratings given to the same samples by a trained panel. Substituting the minimum acceptable liking score in the regression equation allowed estimating the plastic flavor COP. Details of this procedure will be given in the Methods section.

Survival analysis (Meeker and Escobar 1998; Klein and Moeschberger 1997) is a branch of statistics used extensively in clinical studies, epidemiology, biology, sociology, and reliability studies. Hough et al. (2003) introduced survival analysis methods to estimate sensory shelf life based on consumer's acceptance/rejection of aged samples. Consumers receive a set of samples with different storage times and for each one they state whether they accept or reject it. This raw data is analyzed using specialized interval-censored data software to estimate rejection probability as a function of storage time. Based on an adopted rejection probability (usually 50%, Hough (2010)) the sensory shelf life of the product can thus be estimated. The methodology was then extended to estimating concentration limits of sensory defects (Hough et al. 2004) and optimum concentrations of a food ingredient (Garitta et al. 2006). Survival analysis has the advantage that experimental sensory work is relatively simple: a group of consumers answer if they accept or reject samples with different storage times or different levels of a sensory defect. Another advantage is that the accept/reject decision is in line with what consumers do regularly when confronted with a food product close to the end of its SSL or close to intolerable sensory limits. Due to these advantages it would be of interest to use survival analysis methods to establish a sensory COP. As explained in the following paragraph this entails a certain degree of difficulty.

In shelf-life studies the researcher decides at what storage times he/she will extract the samples from their storage conditions. For example, for a yogurt study (Curia et al., 2005), samples were stored for 0, 14, 28, 42, 56, 70, and 84 days. These values are exact, that is there is no doubt that the experimenter extracted samples with 70 days storage, and not 70 ± 2 days. Another example of survival analysis is found in Sosa et al. (2008) who estimated the optimum concentration of salt in French-type bread from a consumer's perspective. They prepared samples of bread with 0.6, 1.2, 1.8, 2.4, 3.0, 3.6, and 4.2 g sodium chloride per 100 g of flour. Since the weighing error of these salt quantities was negligible, the values could be taken as exact as is the case of storage time in a shelf-life study. However, the values of the independent variable may not always be free of error. Consider the case of a yogurt manufacturer interested in estimating shelf lives of present and future formulations. If the critical descriptor has been established as acid flavor, he/she would find it practical to have an acid flavor COP. For any given formulation a correlation would be established between acid flavor and storage time, and with the COP a SSL value could be estimated. To obtain this COP using survival analysis 6-8 samples of yogurt with different levels of acid flavor (prepared, for example, by mixing a highly acid yogurt with different levels of a control sample) would be submitted to a consumer panel and to a trained sensory panel. The consumers would respond if they accept or reject each sample, and the trained panel would measure acid flavor. Nevertheless, trained panel measurements are subject to measurement error. In particular, the mean acid flavor given by the trained panel for one of the samples could be 4.8 on a 1-10 acid flavor scale. However, the acid value assigned to a sample cannot be summarized solely by its mean, its variability has to be incorporated. In the case of the above storage times or grams or salt, variability is null. When a consumer accepts a sample with mean acid value= 4.8 and rejects a sample with mean= 6.2, his/her data is interval-censored (Hough et al. 2003) between 4.8 and 6.2, where these limits are not exact values and their variability has to be taken into account.

Langohr, Gómez and Hough (2013) presented a model to fit parametric distributions to interval-censored data when the interval limits have been measured with certain error. They provide details of the likelihood function corresponding to this data taking into account the variability. The required estimators are obtained maximizing the likelihood function.. Finally, they applied their model to data from a yogurt experiment and estimated the acid taste COP corresponding to various rejection probabilities between 0.1 and 0.9.

The objectives of the present work were: (a) use the recently published survival analysis model (Langohr et al. 2013) to estimate the COP's corresponding to different data sets, and (b) compare the survival analysis COP's with the regression-based COP's (Garitta et al. 2004).

2 Data sets

Three data sets were chosen based on the following criteria:

- Yogurt: a taste descriptor measured by a trained panel was the critical descriptor. The relationship between %Rejection and acid taste was positive.
- Strawberry flavored drink: a flavor descriptor measured by a trained panel was the critical descriptor. The relationship between %Rejection and artificial strawberry was negative.
- Broccoli: the trained panel used a quality index for the appearance of the product. The relationship between %Rejection and quality index was negative.

2.1 Yogurt

Fat-free strawberry yogurts were obtained from a dairy company in Argentina and stored at 10 °C for 0, 14, 28, 42, 56, 70, and 84 d.

Sensory evaluation was conducted using the DESA- ISETA's sensory trained panel (14 women); the resulting critical descriptor was acid flavor which increased over storage time and was measured on a 100-cm structured scale. Consumer testing was performed by 80 regular consumers of the product recruited in the town of 9 de Julio- Argentina. For each sample they were asked "Would you normally consume this product? Yes or No?". They were also asked to evaluate overall acceptability using a 9-pt scale. Details of the experimental procedures can be found in Curia et al. (2005).

2.2 Strawberry flavored drink

Samples of a commercially available strawberry flavored non-carbonated drink were collected from local supermarkets in the UK with different best-before dates. The manufacturer recommended a maximum storage time of 26 weeks; with this information the resulting storage times of the collected samples were: 8, 12, 16, 20 and 28 weeks. It was not possible to have a sample with storage time= 0 as it was not found in the supermarkets.

Sensory evaluation was conducted using the Leatherhead Food Research's sensory trained panel (15 women); the resulting critical descriptor was artificial strawberry flavor which decreased over storage time and was measured on a 10-cm unstructured scale. Consumer testing was performed by 79 non-rejectors recruited from a local data base. They were asked to taste each of the samples and measure their acceptability for: overall liking, appearance and flavor on a 9 pt scale (1=dislike extremely, 9=like extremely). In addition to rating acceptability, consumers were asked if they would accept or reject each sample by indicating 'yes' or 'no' on their ballot form. Details of the experimental procedures can be found in Hough et al. (2013).

2.3 Broccoli

Trays with 300 g of minimally processed broccoli florets were stored at 0ºC for 0, 11, 18, 26, 63, 89, 152 and 169 days. A reversed storage design was used (Hough, 2010) freezing the broccoli trays after each storage time. This allowed the trained panel and consumers to evaluate all samples in a single session at the end of the total storage time.

Sensory evaluation was conducted using the DESA- ISETA's sensory trained panel (10 women); the quality index (QI) method was used to measure the appearance of the product on a 1-6 quality scale. The 1 represented a completely brown broccoli and the 6 a predominantly darkgreen broccoli with small lighter green spots. Details of this scale can be consulted in Garitta et al (2013).

Consumer testing was performed by 81 regular consumers of the product recruited in the town of 9 de Julio- Argentina. Based on the appearance of each tray, consumers were asked if they would normally consume the product (yes/no) as well as their appearance acceptability using a 9-pt scale.

3 Cut-off point calculations

3.1 Regression based COP

The regression-based methodology has been described in detail by Hough (2010). The first step towards estimating a product's sensory shelf life by this method is the determination of the cut-off point which is calculated as follows:

a) Obtain the mean squared error from the analysis of variance on the consumer acceptability rating data and apply the following formula:

$$S = F - Z_{\alpha}\sqrt{\frac{2MSE}{n}} \qquad (1)$$

where:

S = value below which the sensory acceptability of the most preferred sample is significantly reduced;

F = acceptability of most preferred sample;

$Z\alpha$ = one-tailed coordinate of the normal curve for α significance level;

MSE = mean squared error derived from the analysis of variance of the consumer data using consumer and sample as variation factors; and

n = number of consumers.

Basically Equation (1) expresses the difference between acceptability of the most preferred sample and a least significant difference.

b) Correlate the means of the consumer data versus the means of the trained panel data.

c) Perform an inverse prediction by introducing the value of S in the above correlation. If the sensory descriptor is a defect, this will provide the cut-off point above which acceptability is < S. If it is a desirable descriptor, it will provide the cut-off point below which acceptability is < S.

Consumer's ANOVA, correlations and inverse predictions necessary for the regression based COP were calculated using Genstat 15th Edition (VSN International, Hemel Hempstead, U.K.).

3.2 Survival analysis COP

Following, we shall present the main points of the model developed by Langohr et al. (2013) to estimate the COP based on interval-censored survival analysis with variability in the independent variable. To exemplify the presentation, we shall assume the development of acid flavor in yogurt. We denote the distribution function of the random variable T, the acid taste above which yogurts are rejected, by R_T.

Assuming non-informative censoring (Oller et al., 2004) and if the acid tastes were measured without error, the contribution to the likelihood function L_m of subject *m*, whose rejection value lies in interval (Xl_m, Xr_m], would be (Gómez et al., 2009)

$$L_m = R_T\left(x_{r_m}\right) - R_T\left(x_{l_m}\right) \quad (2)$$

However, the exact acid tastes are unknown and estimates obtained from the panel of the trained assessors are given instead. For this reason, we substitute the unknown acid tastes by these estimates and account for the corresponding uncertainty by integrating over the whole range of the estimated mean acid values $\hat{X}_i$, $i = 1, \ldots, I$, which are all real-valued numbers in [0, 100] restricted to $x_{lm} < x_{rm}$. Hence, the likelihood contribution in (2) converts into

$$L_m = \int_0^{100} \int_0^r \left(R_T(r) - R_T(l)\right) dR_{\overline{X}_{l_m}}(l)\; dR_{\overline{X}_{r_m}}(r) \quad (3)$$

Given a sample of size n, (l_m, r_m], m = 1, . . . , n, and assuming independence among the observations, the likelihood function is

$$L = \prod_{m=1}^{n} \int_0^{100} \int_0^r \left(R_T(r) - R_T(l)\right) dR_{\overline{X}_{l_m}}(l)\; dR_{\overline{X}_{r_m}}(r) \qquad (4)$$

In case of left and right-censored observations, that is $l_m = 0$ and $r_m = \propto$, respectively, the likelihood contribution in (3) reduces to the following respective single integrals:

$L_m = \int_0^{100} R_T(r)\, dR_{\overline{X}_{r_m}}(r)$ (left censoring) and $L_m = \int_0^{100} (1 - R_T(l))\, dR_{\overline{X}_{l_m}}(l)$ (right censoring).

We refer to Langohr et al. (2013) for the procedure to maximize the logarithm of the likelihood function (equation 4). The maximization algorithm was implemented by Langohr et al. (2013) in R using different functions of contributed packages. The Weibull distribution is a very flexible right-skewed distribution which is particularly appropriate for modeling survival data and thus it was the chosen parametric distribution. The Weibull rejection probability is given by:

$$R(x) = 1 - \exp\left[-\exp\left(\frac{\ln(x) - \mu}{\sigma}\right)\right] \qquad (5)$$

Where:

R(x)= rejection probability,

x= sensory variable (e g. acid flavor or quality index),

μ= location parameter, and

σ= shape parameter.

4 Results

4.1 Yogurt

Average acceptability of the control sample was 8.4 on a 1-9 scale. The acceptability limit given by Equation (1) was S= 7.9. The relationship of acceptability and acid taste was exponential and given by the following equation:

$$Acceptability = 9.23 - 0.69 \times \exp(0.025 \times acid\ \ taste)$$

The regression was significant (P<0.05) and the regression model explained 96% of the variance. An inverse prediction was performed, entering the regression with an acceptability value of S = 7.9, which gave an estimated cut-off point of 25 on the 0 –100 acid taste scale as shown in Figure 1 (a). This would mean that when the acid taste was greater than 25, there would be a significant decrease in overall acceptability in relation to the most preferred sample. The regression procedure also calculated 95% confidence intervals for the inverse prediction and these were ± 29; being so wide they were not drawn on the COP plot (Figure 1 (a)).

For the survival analysis COP, the Weibull parameters (Equation 5) were μ= 4.177 and σ= 0.243. Figure 1 (b) shows the proportion (%) of rejection versus acid taste. In shelf-life studies a 50% rejection probability has been adopted (Hough, 2010); however, if the COP is to be used for quality control purposes, a 10% rejection probability has been recommended (Hough et al. 2004). The acid taste and the 95% confidence intervals corresponding to 10% and 50% rejection probabilities are shown in Table 1, together with the regression-based COP.

4.2 **Strawberry flavored drink**

Average flavor acceptability of the control sample was 6.0 on a 1-9 scale. The acceptability limit given by Equation (1) was S= 5.5. The relationship of acceptability and strawberry flavor was exponential and given by the following equation:

$$Flavor\ acceptability = 5.27 + 1.68 \times 10^{-6} \exp(0.256 \times strawberry\ flavor)$$

The regression significance level was 0.07, and the regression explained 87% of the variance. An inverse prediction was performed entering the regression with an acceptability value of S= 5.53 which gave an estimated cut-off point of 46 on the 0-100 artificial strawberry sensory scale as shown in Figure 2 (a). This would mean that when the artificial strawberry flavor was below 46, there would be a significant decrease in overall acceptability in relation the most preferred sample. The regression procedure also calculated 95% confidence intervals for the inverse prediction and these were ± 38; being so wide they were not drawn on the cut-off point plot (Figure 2 (a)).

For the survival analysis COP, the Weibull parameters (Equation 5) were μ= 3.941 and σ= 0.228. Figure 2 (b) shows the proportion (%) of rejection versus strawberry flavor. The strawberry flavors and the 95% confidence intervals corresponding to 10% and 50% rejection probabilities are shown in Table 1, together with the regression-based COP. The mean strawberry flavor for the control sample was 50; thus the COP = 62 corresponding to 10% rejection is beyond the experimental range of the samples and thus has no practical value.

4.3 Broccoli

Average acceptability of the control sample was 7.4 on a 1-9 scale. The acceptability limit given by Equation (1) was S= 6.9. The relationship of acceptability and QI was exponential and given by the following equation:

$$Acceptability = 1.74 - 0.001 \times \exp(-1.1 \times QI)$$

The regression was significant (P<0.05) and explained 95% of the variance. An inverse prediction was performed, entering the regression with an acceptability value of S = 6.9, which gave an estimated cut-off point of 5.9 on the 1- 6 QI scale as shown in Figure 3 (a). This would mean that when the QI was lower than 5.9, there would be a significant decrease in overall acceptability in relation to the most preferred sample. The regression procedure also calculated 95% confidence intervals for the inverse prediction and these were ± 0.15.

For the survival analysis COP, the Weibull parameters (Equation 5) were μ= 1.704 and σ= 0.059. Figure 3 (b) shows the proportion (%) of rejection versus QI. The appearance QI and the 95% confidence intervals corresponding to 10% and 50% rejection probabilities are shown in Table 1, together with the regression-based COP.

5 Discussion

For acid flavor in yogurt the regression-based COP was 25 (Figure 1 (a)), while the 10% and 50% survival COP's were 38 and 60, respectively (Table 1). The regression-based COP was based on a significant decrease in acceptability in comparison to the control sample; however it was clear for the yogurt that this decrease in acceptability did not mean product rejection and if adopted would mean a much too conservative COP, leading to unnecessary rejection of samples in quality control or very short shelf-lives. A similar conclusion can be reached with the broccoli results. The 50% survival COP of 5.4 on a 1-6 scale (Table 1) is more realistic than the regression-based COP of 5.9 on a 1-6 scale (Figure 3 (a)). This last value is reflecting a slight decrease in acceptability which has very low rejection probability, approximately 10% as shown in Table 1. Gambaro et al. (2006) compared the SSL of baby food using the COP methodology and survival analysis. When estimating the COP based on a significant reduction in consumer acceptability (Hough et al. 2002) they estimated a SSL of 8 months. The SSL estimated by survival analysis corresponding to a 25% rejection probability was 18 months. Gambaro et al.'s (2006) conclusion was that the COP based on a significant reduction in consumer acceptability can lead to overly conservative SSL estimations. Giménez et al. (2007) in their study on the sensory shelf life of brown bread concluded that using the regression-based COP would be too conservative a criterion to be used by the product manufacturer and therefore the methodology did not apply.

For the strawberry flavored drink the survival COP corresponding to a 50% rejection (Table 1) was similar to the regression-based COP (Figure 2 (a)). Strawberry flavored drink is a product with small batch-to-batch variations and consumers expect constant sensory properties; thus even if a sensory change is small, such as a slight decrease in strawberry flavor, this will probably lead to a significant decrease in acceptability and simultaneous rejection of the product. This could suggest that for products where consumers expect constant sensory properties the regression based COP could be applied. However, the survival analysis approach is sounder.

Regarding confidence intervals, these were very wide for the regression-based COP's in two of the three products (Table 1). Confidence intervals for the survival COP's were within reason and it is expected they will be for other food products. An exception could occur in an experiment in which a large proportion of consumers accepted the product with the highest level of a sensory defect (for example acid flavor in yogurt) or lowest level of a desired sensory attribute (for example strawberry flavor in a drink). A large proportion of consumers accepting these samples would lead to a large proportion of right-censored data which could produce COP estimated with wide confidence intervals. However, this would not be a problem of the survival analysis methodology, rather a problem of inadequate sample preparation.

A question that could arise is what COP values would be obtained by using the mean sensory scores and ignoring variability. These calculations were performed for the three data sets and results were similar to those in Table 1 obtained with the complete model that accounts for variability. However, this similarity in values cannot be guaranteed for all data sets. Having the model and software tools available we recommend the use of the full model.

6 Conclusions

As stated in the Introduction, interval-censored methods have the advantage of being in line with what consumers do regularly when confronted with a food product accept/reject decision, also experimental work is relatively simple. Applying straightforward interval-censored techniques to estimate a sensory COP is not correct due to the uncertainty in the interval limits. Langohr et al. (2013) developed a method which takes this error into account and we have applied this to three food products obtaining COP's for each one. These values were compared to the regression based COP's. For two of the products these last values were unrealistic, and would produce conservative COP estimates, leading to unnecessary rejection of samples in quality control or very short shelf-lives. For one the products (strawberry flavored drink) the survival and regression-based COP's were comparable. Another issue is that confidence intervals tend to be wider for the regression-based COP's than for the survival COP's. As a final conclusion we recommend the survival methodology in estimating sensory COP's as it is based on the consumer's everyday decision to accept or reject food products.

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Figure captions:

Figure 1. (a) Acceptability versus acid taste for yogurt samples. S = value below which the sensory acceptability of the most preferred sample was significantly reduced, this defining the cut-off point (COP) = acid taste above which there was a significant reduction in acceptability. **(b)** Percent rejection versus acid taste for yogurt samples. The dotted lines represent the cut-off point corresponding to 50% rejection with corresponding 95% confidence intervals.

Figure 2. (a) Flavor Acceptability versus strawberry flavor for strawberry flavored drink. S = value below which the sensory acceptability of the most preferred sample was significantly reduced, this defining the cut-off point (COP) = strawberry flavor below which there was a significant reduction in acceptability. **(b)** Percent of rejection versus strawberry flavor for strawberry flavored drink. The dotted lines represent the cut-off point corresponding to 50% rejection with corresponding 95% confidence intervals.

Figure 3. (a) Acceptability versus appearance quality index for broccoli samples. S = value below which the sensory acceptability of the most preferred sample was significantly reduced, this defining the cut-off point (COP) = appearance quality index below which there was a significant reduction in acceptability. **(b)** Percent of rejection versus appearance quality index for broccoli samples. The dotted lines represent the cut-off point corresponding to 50% rejection with corresponding 95% confidence intervals.