

INCORPORATING PRODUCT VARIABILITY INTO QUALITY MODELS

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Keywords: Random Effects, Nonlinear Quality Models, Bootstrap Method, cucumber, mushrooms, tulips

Abstract

An approach is introduced which combines general nonlinear models with fixed cultivar and batch effects for describing quality aspects, with random coefficients to account for differences between individual units within a batch of products. This approach uses least squares to estimate the model parameters and the statistical technique of bootstrapping to obtain confidence intervals around these estimates. This approach enables one to make inferences about the parameters on different levels. Several examples illustrate the wide applicability of this approach.

Introduction

In many agro-research applications, different batches of products (e.g. apples, flowers, mushrooms, cucumbers) are submitted to one of a range of treatments. For example different growing conditions, storage temperatures or process adjustments. One can compare the effect of the different treatments, by monitoring the properties of batches over time. Because of the involvement of complex chemical and physical processes, the behaviour of the items under consideration often is described using nonlinear models with treatment-dependent parameters. Examples in this direction are modelling the loss of firmness of apples, the reddening of tomatoes (Tijskens and Evelo (1994)) and the change of amount of sugar in potatoes.

Generally these quality models in agricultural applications describe the mean behaviour of a batch of products under given conditions. However, a characteristic feature of agricultural applications is the large degree of biological variability between the product units. The individual batch units can exhibit very different behaviour not only due to genetic variation but also through small variations in treatments (position of the plant, the exact amount of nutrition, differences in soil conditions and so on). This variability in product behaviour affects the consumer's perception of the product quality (though not necessarily negatively). Moreover many quality norms are based not on the mean batch behaviour, but on some other feature of the distribution of the property of batch products: a specific quality norm for cucumbers states that no more than 5% of a batch should fall below a certain colour value. Thus information about this variability, in addition to the mean batch behaviour, can enhance the value of the models.

Modelling random behaviour of individual units and the inextricable variability in performance, is the field of statistics. Unfortunately, the benefits of statistics for quality modelling are still often neglected in agro-technological applications, where these benefits just hand a solution to cope with random fluctuations of the objects under study.

In case of repeated measurements of products over time, several statistical methods

already have been proposed to determine the treatment effects. These approaches vary from carrying out an Analysis of Variance for each time point separately, to random effects models (le Cessie and van Houwelingen (1995), Hastie and Tibshirani (1990)). The first method gives rise to a large amount of information which is often hard to interpret. The latter approach seems more suited, but depends heavily upon the assumptions of normality of the data.

The method we present in this paper is not hampered by the aforementioned drawbacks. The model is fitted to the data using least squares regression and the statistical technique of bootstrapping (Efron and Tibshirani (1993)) is used to construct confidence intervals and to make inferences about the parameter estimates. To underline the wide applicability, we illustrate the bootstrap-approach with cases that cover different aspects of agro-production processes, namely growing and production (tulip stem elongation), storage (yellowing of harvested cucumbers) and processing (bottling of mushrooms).

Models and Methods

We deal with individual effects by including them as random coefficients in the nonlinear models. In this way we divide the model parameters into treatment-dependent (batch) parameters and random coefficients that represent the varying effects of the individual batch units. For example, in a model for the change in growth of tulips, the initial vitality of the tulip bulb is a random value, while the rate of growing is treatment-dependent.

The next step is to fit the predescribed nonlinear models to the collected data using nonlinear least squares regression. BCa-bootstrapping (Efron and Tibshirani (1993)) is then applied to estimate the treatment-dependent parameters together with their confidence intervals. These confidence intervals are the basis for inference about the parameter estimates.

The bootstrap

The bootstrap is a computer based statistical technique, which is especially designed to estimate, directly from the available data, the underlying distribution of a predefined estimator or functions of it. Therefore it is ideally suitable for establishing confidence intervals about treatment effects or alternatively about functions of the parameters (for example, with regard to the quality norm). The assumptions on the distribution of the data are very mild; therefore it gives a handle to tackle complex models and incorporate sophisticated optimisation routines. The bootstrap is based on a whole lot of resamples with replacement from the original data set. BCa-bootstrapping corrects for certain deficiencies of the traditional bootstrap method, making it a slightly better method to construct confidence intervals.

On the other hand some warnings apply. A necessary condition to make bootstrapping work is that the estimators of the parameters should be asymptotically normally distributed. For many estimators this is the case but can be very hard or even impossible to verify. Nevertheless, this is a much weaker assumption than the data following a normal distribution. As it is a computer-based method based on a many resamples with replacement from the original data set, bootstrap requires a lot of computer time and memory, especially when combined with computational intensive optimisation programs.

Growing of tulips

The first example concerns the stem elongation of tulips, where the data come from an experiment that monitors the stem length of batches of (6-10) tulip bulbs over

time. There are 135 tulip bulbs in the data set, with a total of 16 different treatments. The treatments applied to the bulbs are combinations of 2 types (A & B) of hormones.

The stem elongation of the tulips $h(t)$ at time t is modelled as (see Wilkinson et al. (1997)):

Equation 1

$$h(t) = \frac{h_{\max}}{1 - (1 - h_{\max}/h_0) \cdot \exp(-rt)} + \varepsilon(t)$$

where we assume the asymptotic stem length ($t \rightarrow \infty$) h_{\max} to be a function of the initial length h_0 at $t=0$ and the applied treatment. The rate constant r is influenced only by treatment and the error is a mean-zero random variable with treatment dependent variance.

Firstly the tulip model is fitted to the data. In this way we can estimate the different model parameters (h_{\max} and r). The treatment dependent variable r is of most interest. Therefore we use the BCa-bootstrap approach to construct confidence intervals around r corresponding with the different treatments. We also pairwise compare the different treatments. If zero is *not* in the approximating 95% confidence interval for the difference of two treatment dependent parameters we may argue that the treatments differ significantly.

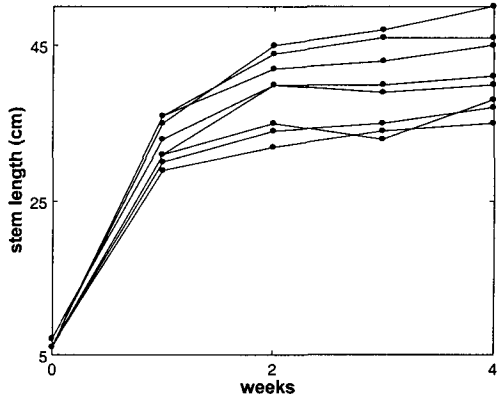


Figure 1 Example data for 1 batch of tulips

Colouring of cucumbers

One of the quality norms on cucumbers concerns the green colour. Schouten et al. (1997) show that the reduction of the amount of green colouring of a cucumber can be modelled adequately using a logistic function of time. The data consists of 62 cucumbers in 4 batches of (10-20) units. The treatments consist of variations in growing conditions. The green colour of the individual cucumbers (= (average red value)/(average blue value) from RGB measurement) is measured repeatedly over time.

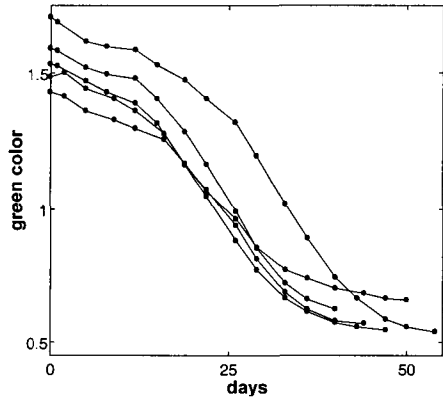


Figure 2 Example data of 5 cucumbers from 1 batch

We can incorporate the individual effects to model the colour $Gr(t)$ at time t in the cucumber as follows:

Equation 2

$$Gr(t) = Gr_{plus} + \frac{Gr_{\min} - Gr_{plus}}{1 + \frac{Gr_{\min} - Gr_0}{Gr_0 - Gr_{plus}} \cdot \exp[tk \cdot (Gr_{\min} - Gr_{plus})]} + \varepsilon(t)$$

Gr_{\min} , Gr_0 and Gr_{plus} indicate the colour at time $t = -\infty$, $t=0$ (the point at which the experiment

begins) and $t=\infty$, respectively. k is the rate constant and $\varepsilon(t)$ is the zero-mean error term which we assume to be independently and identically distributed for each t . Furthermore the model assumes the parameters Gr_{\min} and Gr_0 to be functions of individual (random) and fixed treatment effects, while k is only treatment dependent and Gr_{plus} is a function of the fixed cucumber effect.

Using the BCa-bootstrap we can estimate the parameters and with the model for the green colour of the cucumbers, we can predict the shelf-life \hat{t} , in days, at which 5% of the total batch would reach an (unacceptable) colour level ($Gr=1.202$, which corresponds to the limit of Dutch auction houses).

The model is fitted using nonlinear least squares regression. To investigate the significance of the treatment effects we determine confidence intervals for the estimated parameters \hat{k} . By constructing confidence intervals of differences between the batch parameters for the rate of decolouring k , we can also investigate which pairwise treatments are significantly different. Again, if zero is *not* in the confidence interval, the parameters and therefore the treatments can be judged as significantly different.

Bottling of mushrooms

For the food processing industry it is important to know what is the amount of water a mushroom can hold during the bottling process. An experiment was done concerning the canning of 5 batches of 15 mushrooms each with different process adjustments. The weight of the individual mushrooms was monitored at the beginning of the experiment ($t=0$), after the filling of the cans ($t=1$) and after storage time (drained weight) at ($t=2$).

Unlike the previous cases, we here describe the weight using a nonlinear statistical model instead of a physical model. The weight $w(t)$ at time $t=1,2$ is described as:

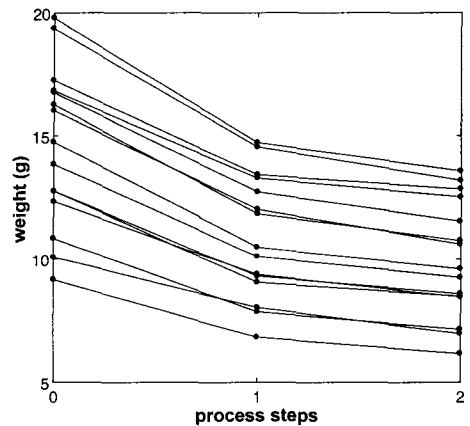


Figure 3 Example data of 1 batch of 15 mushrooms

Equation 3

$$w(t) = w_0 \cdot (\bar{f} + f) \cdot (\bar{d} + d)^{t-1} + \varepsilon(t).$$

w_0 is the weight at the beginning of the experiment (i.e. $t=0$). \bar{f} denotes the average weight rendement ($=w(1)/w_0$) over all batches after the filling process ($t=1$), while f is the additional rendement (which can be either positive or negative) per batch. In the same way \bar{d} is the average weight rendement (over all batches) after draining ($t=2$), relative to $w(1)$, while d is again an additional batch rendement. $\varepsilon(t)$ are again independent zero-mean random variables.

With our approach it is tested whether different treatments give significant differences compared to the average fill rendement and drain rendement. Therefore approximating 95% confidence bounds are constructed using the BCa-bootstrap method, with 1000 samples, for the additional batch effects of different treatments, both for the fill rendement and the drain rendement.

Results

Growing of tulips

At first the tulip model is fitted to the data. From Figure 4, it looks like the model with individual random coefficients describes the data well.

For each batch of tulip bulbs that is submitted to a different combination of the two types of hormones, we construct the approximating 95% confidence bounds for the parameter estimates \hat{r} . The results (Table 1) show that a moderate amount of hormone A gives the fastest stem growth, while addition of hormone B seems to have a positive effect on the stem growth for the low hormone A concentrations.

Table 2 gives the results of testing which treatments are significantly different from each other. These inferences are based on testing whether 0 is in the 95%-confidence region of the difference of the batch dependent parameter estimates \hat{r} (=significant, denoted by 1) or not (= not significant, denoted by 0).

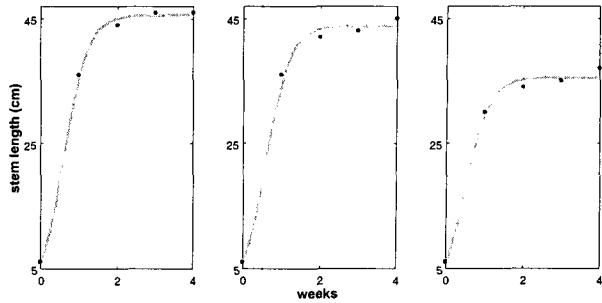


Figure 4 The tulip model fitted to the data of 3 tulips from 1 batch

Table 1 Approximating 95% bootstrap confidence intervals for \hat{r}

batch no.	amount of hormone A	amount of hormone B	95%-conf. interval for \hat{r}
1	0	0	[1.0707 , 1.4076]
2	0.1	0	[1.8813 , 2.4386]
3	0.3	0	[2.4355 , 2.9151]
4	1	0	[2.9422 , 3.1662]
5	3	0	[2.9489 , 3.2400]
6	10	0	[2.9016 , 3.4514]
7	20	0	[3.0118 , 3.3247]
8	30	0	[2.7798 , 3.0759]
9	0	10	[1.0799 , 1.4716]
10	0.1	10	[1.9035 , 2.2198]
11	0.3	10	[2.2916 , 2.6076]
12	1	10	[2.2216 , 2.4356]
13	3	10	[2.4748 , 2.7170]
14	10	10	[2.8237 , 3.1287]
15	20	10	[2.6468 , 3.1535]
16	30	10	[2.9152 , 3.2447]

Table 2 Significance matrix for pairwise differences between treatments

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0	1	1	1	1	1	1	1	0	1	1	1	1	1	1	1
2	1	0	1	1	1	1	1	1	1	0	0	0	1	1	1	1
3	1	1	0	1	1	1	1	0	1	1	0	1	0	1	0	1
4	1	1	1	0	0	0	0	1	1	1	1	1	0	0	0	0
5	1	1	1	0	0	0	0	1	1	1	1	1	0	0	0	0
6	1	1	1	0	0	0	0	1	1	1	1	1	0	0	0	0
7	1	1	1	0	0	0	0	1	1	1	1	1	0	0	0	0
8	1	1	0	0	0	0	1	0	1	1	1	1	0	0	0	0
9	0	1	1	1	1	1	1	1	0	1	1	1	1	1	1	1
10	1	0	1	1	1	1	1	1	1	0	1	1	1	1	1	1
11	1	0	0	1	1	1	1	1	1	1	0	0	0	1	1	1
12	1	0	1	1	1	1	1	1	1	1	0	0	1	1	1	1
13	1	1	0	1	1	1	1	1	1	1	0	1	0	1	0	1
14	1	1	1	0	0	0	0	0	1	1	1	1	0	0	0	0
15	1	1	0	0	0	0	0	0	1	1	1	1	0	0	0	0
16	1	1	1	0	0	0	0	0	1	1	1	1	0	0	0	0

Colouring of cucumbers

Again the model with included individual random parameters seems to explain the data very well. With our method, for each batch of cucumbers (corresponding with different preharvest conditions) the batch dependent parameters \hat{k} together with their confidence intervals are estimated. Furthermore we can estimate the time \hat{t} in days at which 5% of the whole population of cucumbers with that treatment falls below the colour threshold.

We also investigated, just as in the tulip example, which treatments can be viewed as significantly different. It turned out that in this example all treatments are significantly different from each other. This

feature was already somehow indicated by the confidence interval of \hat{k} from table 3. Future research in this direction will be focused on determining the sample size (from which the bootstrap approach resamples) needed to make reliable predictions when a batch will no longer achieve the quality norm on green colour.

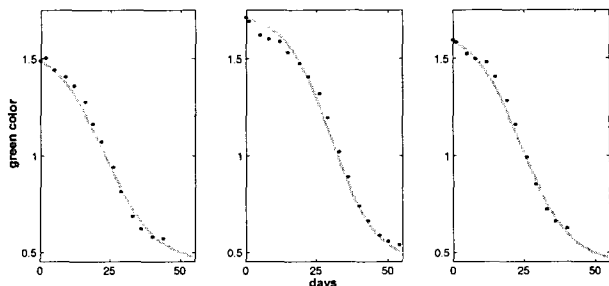


Figure 5 The cucumber model fitted to the data of 3 cucumbers from 1 batch

Table 3 Parameter estimates of cucumber data

batch no.	\hat{k}	95% conf. int. of \hat{k}	\hat{t}
1	0.1288	[0.1262, 0.1300]	13.54
2	0.1190	[0.1179, 0.1199]	13.88
3	0.0969	[0.0946, 0.0976]	13.33
4	0.0944	[0.0917, 0.0957]	16.61

Bottling of mushrooms

For the last example we see that also this nonlinear statistical model fits to the data very well. Furthermore we calculated, with our bootstrap approach for confidence regions, for each batch of mushrooms and process step, whether the corresponding process adjustment gives significantly better or worse results than the mean rendement for each process step.

The indication whether an effect is significantly different from the average rendement is based on the criterion whether 0 is in the confidence interval (significant) or not (not significant) (table 4).

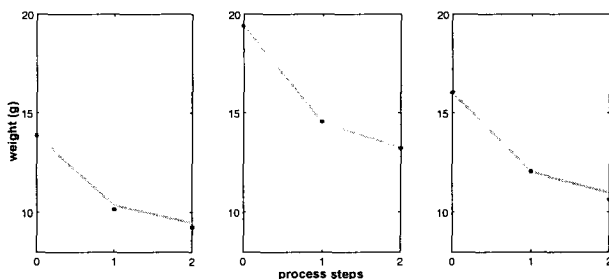


Figure 6 The mushroom model fitted to the data of 3 mushrooms from 1 batch

Table 4 95% bootstrap approximating confidence intervals

batch no.	fill rendement: f	signif.	drain rendement: d	signif.
1	[-0.0417, -0.0125]	x	[-0.0171, 0.0013]	
2	[-0.0345, 0.0022]		[0.0017, 0.0185]	x
3	[-0.0426, 0.0124]		[0.0098, 0.0280]	x
4	[0.0432, 0.0996]	x	[-0.0415, -0.0210]	x
5	[-0.0171, 0.0200]		[0.0001, 0.0187]	x

Conclusions

Nonlinear models with random coefficients representing the individual batch units are widely applicable in agro-technological quality modelling. The main advantage of the proposed bootstrap approach is that it allows one to make statements not only about the mean batch behaviour, but also about many other features of the distribution of the batch units, like variation within the batch in that behaviour. This aspect can have immense value in practical applications (e.g. quality losses in food processing).

Though computer intensive, especially when combined with complex nonlinear models, optimisation algorithms and extensive data sets, the use of bootstrap methods is intuitively appealing for calculating confidence intervals for the treatment dependent parameters based on the variability of the batch units.

This paper indicates that the method is useful for making inference about estimated parameters on different levels. Moreover it reveals that the approach not only works on statistical models (mushrooms) but on physical models (tulips, cucumbers) as well. Also both continuous (tulips, cucumbers) and discrete (mushrooms) models can be tackled, underlining once more the usefulness of our method. These features make the approach very promising for future applications and give plenty of reason for further research.

Acknowledgements

This work uses data provided by Patrick Rietveld and Douwe de Boer (tulips), Rob Schouten (cucumbers) and Eugene Schijvens (mushrooms).

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