Strategies for synchronizing chocolate conching batch process data using dynamic time warping

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Abstract In batch processing, process control is typically carried out comparing trajectories of process variables with those in an in-control set of batches that yielded products within specifications. However, one strong assumption of these schemes is that all batches have equal duration and are synchronized, which is often not satisfied in practice. To overcome that, dynamic time warping (DTW) methods may be used to synchronize stages and align the duration of batches. In this paper, three DTW methods are compared using supervised classification through the *k*-nearest neighbor technique to determine the in-control set in a milk chocolate conching process. Four variables were monitored over time and a set of 62 batches with durations between 495 and 1170 min was considered; 53% of the batches were known to be conforming based on lab test results and experts' evaluations. All three DTW methods were able to promote the alignment and synchronization of batches; however, the KMT method (Kassidas et al. in *AIChE J* 44(4):864–875, 1998) outperformed the others, presenting 93.7% accuracy, 97.2% sensitivity, and 90.3% specificity in batch classification as conforming and non-conforming. The drive current of the main motor was the most consistent variable from batch to batch, being deemed the most important to promote alignment and synchronization of the chocolate conching dataset.

Keywords Batches of variable duration · Phase I of SPC · Dynamic time warping · Chocolate conching · Alignment and synchronization strategies · Batch classification

Introduction

Quality management (QM) practices have become increasingly important in a large number of industrial sectors, being either motivated by rising consumers' expectations, government regulations, or increased market competition. Despite the benefits arising from using such practices, Dora et al. (2013) observed a limitation in the literature addressing QM targeted at requirements from the food sector. Analyzing a sample of micro, small and medium-sized food companies in Europe, the authors found that statistical process control (SPC) was used by only 15% of the companies. That agrees with Lim et al. (2014), who reported an incipient utilization of SPC in food companies when compared to other sectors.

In highly processed food products such as chocolate, the quality of raw materials used in the blend, the proportion in which they are used, and processing conditions are fundamental in establishing the quality of final products (Cidell and Alberts 2006). The chocolate process manufacturing is run in five steps: mixing, refining, conching, tempering and moulding. Chocolate conching is a high investment, time-consuming finite duration batch process carried out in a specific equipment which vigorously mixes components during 5 h to 3 days under increasing temperature from 45 to 80 °C in batches of 2 to 20 tons (Bolenz et al. 2003, 2008, 2014; Di Mattia et al. 2014; Franke and Tscheuschner 1991; Owusu et al. 2012; Torres-Moreno et al. 2012). The conching step is divided in 4 phases; namely: (1) feeding, (2) dry conching, (3) plastic

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conching, and (4) liquefaction. In the feeding phase, refined chocolate is loaded in the conche and temperature is raised up to 45 °C. Emulsifiers may be added at this phase to give the chocolate mass a smoother structure, but they are often added at the liquefaction phase. Dry and plastic conching take place in the main conching phase. During dry conching the chocolate mass is mixed under high temperature (70–80 °C), and the louvres (upper windows of the conche) are maintained opened to allow evaporation of water and undesirable volatile acids, while aeration of product takes place (Bolenz et al. 2003, 2008; Bühler 2010; Prawira and Barringer 2009). Transition to plastic conching starts when fat and/or soybean lecithin emulsifier are loaded (Bolenz et al. 2003; Glicerina et al. 2015). At this point, the current dependent drive changes from clockwise to anti-clockwise rotation in order to continue intense shearing and ensure better fat incorporation in the chocolate mass. Liquefaction phase starts when chocolate mass temperature is reduced to 45 °C, and vanilla flavor and emulsifiers (soybean lecithin and/or polyglycerol polyricinoleate) are added while intense shear is applied. To prevent the mass from splashing out of the conche and to mix additives, louvres are closed and the rotation speed of shovels is reduced. Upon conclusion of this phase, a fluid chocolate mass should be available with rheological properties that ensure the efficiency of remaining process steps (such as pumping, tempering, and moulding) and sensory characteristics (such as consistency, smooth texture, melting, mouthfeel, and snap) (Afoakwa et al. 2008; Bolenz et al. 2003; Bühler 2010; Franke and Tscheuschner 1991; Glicerina et al. 2013; Owusu et al. 2012; Prawira and Barringer 2009). To verify that, a sample of the mass is collected, and its rheological parameters are assessed. If results are in accordance with a required quality specification the batch is classified as conforming; otherwise, a new addition of emulsifiers or fat is usually required to correct the chocolate mass' rheology and the batch is classified as non-conforming.

During conching a large number of process variables are monitored; e.g. rotation speed of shovels, drive current of the main motor, and chocolate temperature (Bühler 2010). Processing variations, particularly in batch temperature profile and duration, may lead to several quality problems in the final product; e.g. heterogeneous and unsmooth chocolate, absence of desirable flavors or presence of acid flavor, fatty mouthfeel, fat and sugar bloom, and abnormal viscosity, texture and chocolate flavor. Thus, time/temperature settings are important process parameters, acting as indicators of the chocolate's final quality (Cidell and Alberts 2006; Di Mattia et al. 2014; Prawira and Barringer 2009; Torres-Moreno et al. 2012). However, process variables are rarely used to predict the product's final quality, which is often assessed by physicochemical analysis after

the product has been sent to the next processing step (Kassidas et al. 1998). As a consequence, the quality control may become inefficient generating a high level of non-conforming products. Aiming for better results, a monitoring based on a SPC method should be implemented.

Process monitoring in SPC is carried out in two phases. In Phase I historical past batches classified as conforming by the industry are tested using the control charts to verify process stability. Batches falling within charts' control limits are used to develop an appropriate in-control model. In Phase II, control charts parameterized using the in-control model are used to monitor future batches, with process data collected successively over time to identify abnormal process behaviors, which causes non-conforming batches (fault detection). Whenever a control charts signals an out-of-control situation process variables contributing most to the fault are identified (fault isolation), and the root cause of the observed out-of-control status is determined (fault diagnosis). Finally, fault effects are removed from the data (process recovery) (Kuang et al. 2015; Woodall and Montgomery 2014). Batch process monitoring using control charts relies on the in-control model's ability to discriminate between conforming and non-conforming batches. Therefore, the correct classification of batches in the dataset used to obtain the in-control model determines its quality.

The use of principal component based control charts to allow on-line and off-line monitoring of a massive amount of data emerging from multivariate batch processes, such as chocolate conching, has been extensively investigated (Jackson and Mudholkar 1979; Kourti and MacGregor 1996; MacGregor 1997; Nomikos and MacGregor 1994, 1995). All schemes are based on the use of multiway principal components analysis (MPCA) to promote dimensionality reduction of process datasets. Such reduced data are then used to construct control charts that allow verifying the behavior of a new batch in the fault detection Phase II step of SPC.

A main assumption constrains the use of MPCA-based control charts for batch process monitoring: all batches considered in the analysis must present the same duration, and be synchronized with respect to process stages (González-Martínez et al. 2011; Kassidas et al. 1998; Ramaker et al. 2003). That is rarely the case in datasets obtained from the conching step of chocolate processing. The typical time required to conch different types of chocolate may vary due to a number of factors; namely: (1) environmental, such as room temperature and humidity; (2) operational, such as high feeding time of the conche, closed louvres during dry conching phase, and unplanned interruptions in processing; and (3) quality-related, such as high moisture content of raw materials, variation due to cultivar,

agricultural practices, soil, climate, etc. These factors cause the duration of batches to vary, and limit the application of MPCA-based control charts in the conching process.

To overcome that, batch process datasets must be pretreated before process modeling and monitoring; for that, methods that align and synchronize variables' trajectories (García-Muñoz et al. 2003) are used such that all batches display the same duration. Direct signal synchronization methods are based on signal processing strategies to align and synchronize batches' profiles, such as (1) truncating trajectories of all batches to match with the shortest one (Kourti 2003a), (2) using an indicator variable other than the time index to rescale process trajectories such that they display the same length (Nomikos and MacGregor 1995) and (3) using methods based on warping techniques, such as dynamic time warping (DTW) (Kassidas et al. 1998) and its improved versions (Ramaker et al. 2003; González-Martínez et al. 2011). In general, the uneven-length phenomenon may occur in one or several operating stages (Lu et al. 2004); thus, truncating trajectories may lead to loss of important information about sources of batch variation. To use the indicator variable proposition, a priori process knowledge must be available such that the variable may be identified. That may be challenging since the indicator variable meets some requirements such as progress monotonically in time and have the same starting and ending value for each batch. DTW methods promote alignment and synchronization by appropriately translating, expanding, and compressing local segments of two trajectories (i.e. a random batch trajectory in the dataset and a predefined reference batch trajectory) to achieve the minimum distance between them. DTW methods have the advantage of using the information of the complete dataset maintaining its time index, which is important for a better interpretation of final process monitoring results. Kassidas et al. (1998) were the first to present an iterative method based on DTW for the synchronization of batch trajectories from an industrial emulsion polymerization process before the application of Nomikos and MacGregor (1994, 1995)'s MPCA-based monitoring scheme. Subsequently, improved DTW methods were published (Ramaker et al. 2003; González-Martínez et al. 2011). However, different DTW methods may lead to different sets of synchronized batches, and that may impact the performance of monitoring schemes, particularly with respect to the determination of the in-control set of conforming batches.

The objective of the present study is to compare different methods for the alignment and synchronization of batch process datasets with varying duration using DTW. Methods are compared regarding their ability to correctly classify batches of a milk chocolate dataset as conforming

and non-conforming. Based on classification performance metrics the most adequate method to pre-treat the dataset is defined, allowing the development of a robust in-control model (Phase I of SPC) with respect to which future batches will be compared (in Phase II) and enabling a more efficient decision-making on process stability and the quality of its outputs. To the best of our knowledge, no previous work addressed this problem.

SPC implementation in batch processes is of utmost practical importance since process performance could be monitored throughout the batch progression, and its accordance to quality standards could be assessed at the end of the batch without relying on final products' lab analyses. Physicochemical analyses would be carried out only when process control charts signalize a non-conforming batch, minimizing quality control efforts. It is not our goal to identify types of variations (e.g. due to raw materials or industrial equipment) causing batches to vary in duration; knowing that in practice most industrial batches display different lengths, our goal is to identify which alignment and synchronization method leads to a better Phase I in-control model development.

Materials and methods

Alignment and synchronization of batches is a data pre-treatment step required for SPC implementation. As shown in Fig. 1, the chocolate conching dataset is comprised of J process variables measured at K time intervals in I batches, and may be organized as a three-way data matrix $\mathbf{X}(I \times J \times K)$. Even if the expected batch duration is known beforehand industrial batches rarely finish at the exact same time instant. Therefore, before implementing SPC the tridimensional dataset (comprised of batches with variable duration) requires a pre-treatment step, as follows: (1) dataset unfolding, (2) treatment of missing values and (3) outliers, and (4) alignment and synchronization of batches' lengths. This section will present the analyzed chocolate conching dataset, pre-treatment steps and the k NN classification technique used for comparison of 3 different DTW methods.

Chocolate conching dataset with batches of variable duration

Data from 69 conching batches of milk chocolate processed between April 2014 and January 2015 were collected from 2 industrial conches (Bühler AG, Uzwil, Switzerland) in a chocolate manufacturing plant located in the south of Brazil. The expected batch duration for this type of chocolate is 495 min, but the sample

Fig. 1 Statistical process control of a chocolate conching dataset

contained uneven-length batches which took up to 1170 min to completion. The dataset included conforming and non-conforming batches, which were classified according to off-line analyses of viscosity and yield value. Fineness and moisture content were also evaluated by the Quality Control department. Results of measurements were obtained 5 min (fineness) and 15 min (viscosity and yield value) after sample collection, allowing corrections before the batch was sent to the moulding lines. Conching duration above the expected value usually occurs when rheological specifications are not achieved, requiring corrections in the chocolate mass. Moisture measurements were not considered for batch classification, since results were not available before 2 days after sample collection (note that abnormal moisture results could point to raw materials out of specification or to the occurrence of water leakage in the conching equipment; in addition, in case of high final moisture content rheological results will be impacted leading to an increase in viscosity values).

Among the several process variables observable during conching, experts recommended monitoring four which are strongly related to chocolate output's rheology; namely: (1) chocolate temperature, which is also related to chocolate flavor; (2) drive current of the main motor, (3) speed of shovel, and (4) frequency of soybean lecithin dosage.

Statistical process control applied to a chocolate conching dataset

Real datasets bring a new layer of complexity to data analyses, usually requiring adjustments before statistical methods can be correctly implemented. In this sub-section pre-treatment steps carried out in the milk chocolate conching dataset are described. The Phase I and Phase II implementation of SPC are not detailed since they are not the subject of the present paper.

Dataset unfolding

The concept of batch-wise unfolding described by Kourti (2003b) was adopted here, resulting in a two-dimensional matrix ($I \times JK$), where each row corresponds to a batch. As described by Nomikos and MacGregor (1995), batch-wise unfolding is recommended when the objective is batch process monitoring with SPC methods.

Missing values

Variables were measured every 60 s as batches progressed. Missing observations occurred when sensors started registering data at different moments or when measurements

were not taken due to sensor failure. Missing values were treated as follows: (1) when a missing observation (or sequence of missing observations) displayed equal values in the immediately preceding and subsequent entries, missing observations were replaced by that value; (2) when a missing observation displayed different values in the immediately preceding and subsequent entries, it was replaced by the average of those values; and (3) when a sequence of missing observations displayed different values in the immediately preceding and subsequent entries, missing observations were replaced by values that gradually increased/decreased, obtained by linear interpolation. The largest sequence of missing observations found in the dataset corresponded to 3 min.

Outliers elimination

From the set of 69 batches, 7 were excluded for presenting drive current and speed readings larger than the maximum admissible values informed by the conching equipment manufacturer. The outlier batches were identified plotting the original data as a function of time (data not shown) and usually occurred before or after a missing value, indicating that it was the result of sensor failure.

Alignment and synchronization of multivariate batch datasets

Three alignment and synchronization methods were applied to the milk chocolate conching dataset. They were all comprised of a symmetric DTW algorithm followed by an asymmetric synchronization procedure. The three methods were proposed by Kassidas et al. (1998), Ramaker et al. (2003) and González-Martínez et al. (2011), respectively, and denoted hereafter as KMT, RSWS, and GFW.

The main principle of DTW is the non-linear warping of pairs of trajectories such that similar events are aligned and the best path through a grid of vector-to-vector local distances is found, minimizing the total distance between trajectories. The local distance used is the weighted quadratic distance, given in Eq. (1) (Kassidas et al. 1998).

$$d(i(k), j(k)) = [\mathbf{B}_t(i(k), :) - \mathbf{B}_r(j(k), :)] \times \mathbf{W} \times [\mathbf{B}_t(i(k), :) - \mathbf{B}_r(j(k), :)]^T \quad (1)$$

where $i(k)$ denotes the trajectory data vector for batch $\mathbf{B}_t$, $j(k)$ denotes the trajectory data vector for reference batch $\mathbf{B}_r$, and $\mathbf{W}$ is a diagonal matrix of relative importance weights for each variable at the next iteration (Kassidas et al. 1998).

Figure 2 shows the optimal path obtained minimizing the weighted local distance between $\mathbf{B}_t$ with duration I and $\mathbf{B}_r$ with duration V . For alignment and synchronization, the average of points in the same line is calculated, and points in the same column should have their values repeated in order to obtain a final batch $\mathbf{B}_t$ with the exactly same duration as $\mathbf{B}_r$.

The main difference between the 3 DTW methods is in the definition of $\mathbf{W}$ matrix. In KMT the weights are computed to provide an indication of which process variables are consistent from batch to batch, and synchronization of batch trajectories relies on those variables. In RSWS matrix $\mathbf{W}$ indicates which variables contain more warping information, explaining main occurrences in the process. It is clear that KMT and RSWS are grounded on different interpretations of weights and may lead to different warped datasets. Finally, GFW pursues a balance between the KMT and RSWS methods, defining a $\mathbf{W}$ matrix in which higher weights are assigned to variables that are consistent from batch to batch, while simultaneously providing meaningful warping information.

Fig. 2 Dynamic time warping strategy for alignment and synchronization of batches of uneven lengths

All batches (conforming and non-conforming) were aligned and synchronized with respect to a B_r such that all batches display the duration of b_r , as shown in Fig. 2. The choice of B_r is another point of difference between DTW methods. In KMT and RSWS, B_r corresponds to the batch with duration closest to the average duration of conforming batches; in GFW B_r corresponds to the batch with duration closest to the median duration of conforming batches.

In this paper, two adaptations were implemented in the methods above. First, the band global constraint (Fig. 2) was not used. Such constraint aims at speeding up computational time by excluding certain regions of the dataset in which the optimal path may lie. This is particularly important in on-line applications; however, as analyses were conducted off-line the main goal is to find the optimal path across all batches and computational time became a minor issue. Second, a new convergence criterion for the weight matrix W is proposed. In this study, the iterative procedure was stopped when the difference between each variable weight in the current iteration and the ones in the immediately previous iteration was smaller than $|0.0010|$. Evaluation of results after weights achieved the convergence threshold showed that they were not significantly improved.

The alignment and synchronization methods tested were implemented in MATLAB R2012b; all codes are available upon request. Detailed information about each method could be obtained in Kassidas et al. (1998), Ramaker et al. (2003) and González-Martínez et al. (2011).

Comparison of DTW methods using the kNN classification technique

The k -nearest neighbor (kNN) classification technique (Bhatia and Vandana 2010; Cover and Hart 1967; Duda et al. 2001) was used to evaluate the classification performance of aligned and synchronized batches given by each DTW method. The treated supervised dataset is comprised of process variables data (X) and a binary output variable (Y), which assumes values 0 (non-conforming class) or 1 (conforming class). For a given batch, using classification performance metrics (accuracy, sensitivity, and specificity), the kNN technique compares the class to which the batch was assigned considering the predominant class of its k -nearest neighbors (i.e. with the smallest Euclidean distance from the analyzed batch), with the classification provided by the industry. For example, if 2 of the 3 nearest neighbors ($k = 3$) of a new batch are conforming, then the batch will be classified as conforming. To avoid ties, k is any positive integer odd value.

The treated supervised dataset, was partitioned such that 80% of the data were used as training portion, and 20% as

test portion. Five different odd numbers of neighbors ($k = 1, 3, 5, 7$, and 9) were tested and the best value of k was selected as the one that achieved the highest average classification accuracy in the test portion (in case of tie, the smallest k was chosen). Average accuracy was computed based on 100 iterations, being given by the number of correctly classified batches divided by the total number of classifications (Anzanello et al. 2009). Sensitivity and specificity values were also computed for each value of k . Sensitivity corresponds to the *true positive rate* (i.e. the number of true conforming batches divided by the total number of batches classified as conforming), and specificity is the *true negative rate* (i.e. the number of true non-conforming batches divided by the total number of batches classified as non-conforming) (Alpaydin 2010).

Since the objective is to refine the definition of the in-control set of conforming batches to be used in Phase I of SPC, the DTW method with largest values of classification accuracy and sensitivity was deemed best for the milk chocolate dataset under analysis. Specificity is also particularly relevant in situations where the focus is to minimize unnecessary production line interruptions and financial losses. The kNN was implemented in MATLAB R2012b; codes are available upon request.

Results and discussion

Three DTW methods were applied to promote the alignment and synchronization of batches in a milk chocolate conching dataset. Process experts selected four process variables to be monitored, with observations available at each minute. Variable $MS6$ ('Metering System #6') shows the frequency of soybean lecithin dosage; variables S ('speed') and DC ('drive current') give the rotation speed of the shovels and current of the main motor that promotes the rotation of the conche axis; variable CT ('chocolate temperature') gives the temperature of the mass during conching.

The dataset was pre-treated resulting in 62 batches classified as conforming (53%) and non-conforming (47%). Classification is an input of the DTW methods since the reference batch (B_r) is chosen from the subset of conforming batches. Pre-treated variables were scaled according to their average range, in all DTW methods, resulting in plots shown in Fig. 3. Variable $MS6$ displays occasional step changes in its level, being suitable to test the quality of synchronization. Variables S , DC and CT , although noisy, display an identifiable shape along the batch duration, proving that outliers were successfully removed. Differences in duration and lack of synchronization across batches may also be verified.

Fig. 3 Scaled pre-treated variables before synchronization

As previously mentioned, the choice of B_r varied according to the DTW method being tested. The final length of batches treated by KMT and RSWS was 716 min, and the corresponding three-way warped data matrix had 177,568 data points. In GFW the length of batches was warped to 699 min, and the corresponding three-way data matrix had 173,352 data points.

Convergence criteria varied according to the DTW method under test. The number of iterations required per method was 29 for the KMT, 34 for the GFW, and 36 for the RSWS. On average, 36 min were required to perform an iteration of the methods. Figure 4 shows the results of alignment and synchronization of batches obtained using each method. All methods were able to promote the synchronization of batches with similar results. Profiles of aligned and synchronized variable *MS6* obtained by KMT and RSWS were very similar, with small differences at the end of batches. The synchronization promoted by GFW differs from the other methods both in the duration and phase change points, which may be explained by the choice of B_r ; its shape and synchronization results, however, are very similar to the other methods.

Profiles in Fig. 4 allow identifying the progression of four industrial chocolate conching phases: feeding, dry conching, plastic conching, and liquefaction (Bühler 2010). From the profile of variable *MS6* two additions of soybean lecithin emulsifier were identifiable: at minutes 19 and 496 for KMT and RSWS, and at minutes 18 and 435 for GFW. The first addition took place at the beginning of the feeding phase, and the second at the beginning of the liquefaction phase. Smaller step changes noticeable at the end of batches were related to lecithin additions aiming at correcting viscosity and yield values of non-conforming batches.

Analyzing the profile of variable *DC*, the end of the chocolate feeding phase took place at minute 81 (for KMT and RSWS) and minute 91 (for GFW), when power increase reaches a plateau. Simultaneously, several

oscillations in speed were observable at the beginning of batches analyzing variable *S* until a maximum permissible speed plateau was reached, favoring an adequate refined mass distribution in the conche as feeding occurs. During dry conching phase, at minute 115 (for KMT and RSWS) speed was reduced to ensure an adequate mass aeration. At minute 209 vegetable fat was added and the speed increased to allow plastic conching to occur, when kneading of the chocolate mass was required to better incorporate the fat. The power (variable *DC*) remained high and constant until the current dependent drive changed rotation from clockwise to anti-clockwise at minute 274 (for KMT and RSWS). Speed remained high and the power started to decrease, as the chocolate mass needed progressively lower power to knead. When the mass was sufficiently liquid, speed and power decreased to lower the shear as the chocolate mass was now very soft and offered little resistance to the conching tools (such speed reduction also avoided the liquid mass to splash out of the equipment).

Soybean lecithin was then added to the mass at minute 496, starting the liquefaction phase. Variable *S* displayed a peak at this point since intense shear was required to properly mix emulsifiers into the chocolate mass. In the GFW method, the behavior of variables *S* and *DC* was not so obvious; however, rotation changeover and speed reduction at the end of the plastic conching were observable after minute 265 of processing. The temperature got higher when the feeding phase ended and should reduce when the liquefaction phase started; however, variable *CT* did not show clearly such temperature variations in any of the methods analyzed.

Figure 5 showed the progression in variables' weights as iterations of the DTW methods took place. At the start of the synchronization procedure it was not possible to average the batch trajectories since they had different durations, so W was assumed to be an identity matrix. From the

Fig. 4 Variables' profiles after synchronization using (a) KMT (Kassidas et al. 1998) (top), (b) RSWS (Ramaker et al. 2003) (middle), and (c) GFW (González-Martínez et al. 2011) (bottom) methods

fourth iteration on, the $\mathbf{W}$ matrix considered the average trajectory batch to be $\mathbf{B}_r$. That explains the variation in weights in early iterations.

Depending on each method's objective in considering $\mathbf{W}$ in the warping process, different information is extracted from the synchronization.

Variable DC is the one with higher increment in synchronization capability if weights of the KMT method are analyzed, representing 52.19% of the total weight at the final iteration, and deemed the most consistent variable from batch to batch. That is evident in variable DC 's profile in Fig. 4. On the other hand, variable DC was not efficient in explaining the main occurrences in the process, representing only 3.45% of the total weight in the RSWS method. Variables S and $MS6$ presented some dispersion between synchronized batches, being assigned lower weights than DC (22.05% and 20.21% respectively).

Finally, variable CT was the most dispersed across batches (represented by a large variation band in Fig. 4), being assigned the lowest weight in KMT method (5.55%).

In the RSWS method the largest weight is assigned to the variable with largest dispersion across batches. Thus, variable CT was the one with highest warping information, accounting for 82.95% of the total weight. All other variables displayed lower weight values, since their deviation from average trajectory was smaller. Variable DC displayed the lowest weight (3.45%).

In the GFW method weights were distributed in a narrower range: from 28.8% (variable $MS6$) to 20.12% (variable CT) due to a better balance between consistency and warping information promoted by the method.

Results in Fig. 4 suggest that synchronization may be dependent on the choice of $\mathbf{B}_r$. To check that, the outputs of all methods implemented with the same $\mathbf{B}_r$ were evaluated

Fig. 5 Percentage of total weight per iteration number by (a) KMT (Kassidas et al. 1998) (top), (b) RSWS (Ramaker et al. 2003) (middle), and (c) GFW (González-Martínez et al. 2011) (bottom) methods

(data not shown). First, KMT and RSWS were run using B_r proposed in GFW (i.e. the batch with duration closest to the median duration of conforming batches); then, GFW was run using B_r proposed in KMT and RSWS (i.e. the batch with duration closest to the average duration of conforming batches). Results showed that the choice of B_r defines the length and phase changing points of synchronized trajectories, but do not impact on the quality of synchronization or the importance of variables in W matrix (the most consistent variable in KMT and the variable with the most warping information in RSWS remains the same, regardless of B_r). Batches synchronized with the shorter trajectory length (699 min) required more iterations to convergence than batches synchronized with the longer trajectory length (716 min). That suggests that number of iterations is not directly related to length, but to shape and dispersion of the chosen B_r .

In addition to evaluating synchronization performance, the goal is to verify how each DTW method affected the classification of synchronized batches in conforming and non-conforming. The kNN classification technique was

chosen for that. First, the dataset of synchronized batches was split into training and test portions, and the influence of the number of iterations in the final classification was evaluated. When performing 100, 200, 300, 400 and 500 iterations of the kNN the resulting standard deviation of average accuracy, sensitivity and specificity was lower than 0.7%, and the difference in performance as a function of the number of iterations was deemed not significant. Therefore, to minimize computational effort, analyses reported next resulted from running 100 iterations of the algorithm.

Running the kNN algorithm in the test portion of the chocolate conching dataset, varying parameter k from 1 to 9, the values of average and standard deviation for three classification performance metrics were obtained: accuracy, sensitivity, and specificity. Results are given in Table 1. In the conching process, accuracy of classification is of major importance: correct classification of batches is key to an adequate SPC. A higher specificity value is also crucial to avoid that non-conforming batches are misclassified as conforming, and released to the moulding lines.

Table 1 Classification accuracy, sensitivity, and specificity for synchronized batches; all values given in percentage

	KMT method					RSWS method					GFW method				
	<i>k</i>					<i>k</i>					<i>k</i>				
	1	3	5	7	9	1	3	5	7	9	1	3	5	7	9
Accuracy															
Average	93.5	93.7	91.4	90.8	90.3	91.6	90.9	90.3	88.8	87.9	89.6	91.3	92.0	92.0	91.3
Standard deviation	6.9	6.5	8.0	8.6	8.7	6.5	7.3	7.1	8.6	8.9	7.9	7.1	6.9	7.3	7.7
Sensitivity															
Average	96.0	97.2	95.8	94.9	93.2	95.4	97.0	95.3	93.3	91.4	90.6	95.4	96.6	97.8	97.9
Standard deviation	9.1	6.5	7.5	8.3	9.5	8.3	6.5	8.3	9.2	9.9	11.5	8.1	7.4	5.3	5.1
Specificity															
Average	91.4	90.3	87.6	88.1	88.7	88.3	84.6	85.9	85.3	85.2	88.8	87.5	87.7	86.8	85.3
Standard deviation	11.6	12.0	14.2	14.5	15.0	13.1	14.8	13.5	15.2	15.4	12.0	12.6	12.5	13.3	15.0

As batches are classified according to rheological parameters, a low specificity potentially leads to a number of technical problems in the process, such as imperfect covering of bonbons, poor spreading of chocolate mass in bar moulds, and blocking of pipes and moving parts of the moulding equipment requiring interruptions in the production line for cleaning and disposal of products. That results in time and financial losses to the manufacturer. On the other hand, high sensitivity values are desired to better define the set of conforming batches to be used in the development of the monitoring in-control SPC model. The KMT method with $k = 3$ was selected as the one with the best combination of classification performance metrics. It yielded the highest average accuracy across methods and the second higher sensitivity and specificity average values. The RSWS method attained good results for $k = 1$, however with lower accuracy, sensitivity and specificity average results than the KMT method. Analyzing these results, it is possible to conclude that the choice of DTW method influence the ability of classifying batches in conforming or non-conforming.

RSWS' specificity with $k = 1$ resulted 2% lower than that of the KMT method with $k = 3$. Considering the number of batches processed in the plant analyzed, that corresponds to the misclassification of 2 batches per year; i.e. using the RSWS method to obtain the reference distribution to be used in SPC would imply in 12 tons of non-conforming chocolate mass being wrongly sent to the production line, leading to a series of technical problems. Losses will be greater proportionally to the deviation of the chocolate mass viscosity from its target value. Given that the milk chocolate mass is used in the production of bonbons, and that non-conforming masses force the production line to halt, that would represent a total financial loss of US\$ 1700.00 in labor, and of US\$ 17,000.00 in raw materials.

In the analyzed plant, 47% of the produced batches required some sort of correction. The average time to correct non-conforming masses was 52 min; assuming that production batches were expected to last average 495 min, 2 out of 18 planned batches were not produced due to such corrections. In addition, extra expenditure with raw materials required to correct non-conforming masses (e.g. soybean lecithin and vegetable fat) were also relevant, amounting to US\$ 7500.00 per year. The described losses in processing time and raw material can be substantially minimized by correctly implementing SPC in the conching equipment.

In terms of chocolate mass quality, the high number of non-conforming batches (47%) reflects the inadequacy of strictly assessing chocolate mass quality after batch completion through lab tests. Aiming at a more efficient quality control, the proposed solution is to implement SPC in the studied process with the development of a more robust in-control model for Phase I of SPC. For that, we propose the use of the k NN classification technique to identify the most adequate DTW method for the pre-treatment of a chocolate conching dataset comprised of batches with variable duration, aiming at a more accurate in-control model and potentially leading to a reduction in the number of non-conforming batches produced. In addition, implementing multivariate SPC methods through MPCA-based control charts allows identifying the time instants in batch progression in which deviations in variables' expected trajectories are more likely to result in non-conformities. Such knowledge simplifies the practice of process control helping operators to focus on key moments in batch evolution. Acting correctively on the process when SPC-controlled variables deviate from their expected trajectories avoids producing non-conforming batches that will latter require correction leading to higher production costs and losses.

The *kNN* technique was also run to evaluate if different choices of B_r had an influence on the correct classification of batches (data not shown). When B_r was not the one suggested in the original DTW method, more k neighbors were required to obtain similar classification performance results. For example, when KMT used B_r suggested in the original method, 3 neighbors were required to obtain the highest accuracy (93.7%); on the other hand, when using B_r recommended in GFW 7 neighbors were required to obtain similar accuracy (93.3%). The same occurred with RSWS and GFW.

Correct classification of batches is key when determining the reference distribution of conforming batches to be used in SPC. With that in view, KMT was deemed the most adequate DTW method to promote alignment and synchronization of batches in the chocolate conching dataset: it was the method that least affected *kNN*'s ability to correctly classify batches in conforming and non-conforming classes. Due to its consistency, variable *DC* was deemed the most important to promote the alignment and synchronization of the chocolate conching dataset.

Conclusion

In chocolate manufacturing process, batches typically do not present the same duration. As a consequence, traditional techniques as MPCA-based charts are not suitable for process control and monitoring. To address that issue, this paper compared three DTW methods that align and synchronize process variables' trajectories aimed at properly determining the reference distribution for multivariate SPC. Findings suggested the KMT method as the best DTW option for aligning and synchronizing a milk chocolate conching dataset. Such method was recommended due to the lowest number of iterations required to achieve convergence and highest average accuracy in the testing portion using the *kNN* classification technique. Future research includes the development of approaches focused on dimension reduction of datasets through variable selection, the implementation of Phases I and II of the SPC in the pre-treated chocolate conching dataset, and the stratification of causes of non-conforming batches in those due to process equipment and due to raw materials, in order to improve the understanding about the sources of process variability.

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References

- Afoakwa EO, Paterson A, Fowler M, Vieira J (2008) Relationship between rheological, textural and melting properties of dark chocolate as influenced by particle size distribution and composition. *Eur Food Res Technol* 227:1215–1223
- Alpaydm E (2010) Introduction to machine learning. The MIT Press, Cambridge
- Anzanello MJ, Albin SL, Chaovalitwongse WA (2009) Selecting the best variables for classifying production batches into two quality levels. *Chemom Intell Lab Syst* 97:111–117
- Bhatia N, Vandana A (2010) Survey of nearest neighbor techniques. *Int J Comput Sci Inf Secur* 8(2):302–305
- Bolenz S, Thiessenhusen T, Schäpe R (2003) Fast conching for milk chocolate. *Eur Food Res Technol* 218:62–67
- Bolenz S, Kutschke E, Lipp E (2008) Using extra dry milk ingredients for accelerated conching of milk chocolate. *Eur Food Res Technol* 227:1677–1685
- Bolenz S, Manske A, Langer M (2014) Improvement of process parameters and evaluation of milk chocolates made by the new coarse conching process. *Eur Food Res Technol* 238:863–874
- Bühler A (2010) Operating Instructions ELK/DÜC conches. Uzwil, Switzerland
- Cidell JL, Alberts HC (2006) Constructing quality: the multinational histories of chocolate. *Geoforum* 37(6):999–1007
- Cover TM, Hart PE (1967) Nearest neighbor pattern classification. *IEEE Trans Inf Theory* 13(1):21–27
- Di Mattia C, Martuscelli M, Sacchetti G, Beheydt B, Mastrocola D, Pittia P (2014) Effect of different conching processes on procyanidin content and antioxidant properties of chocolate. *Food Res Int* 63:367–372
- Dora M, Kumar M, Van Goubergen D, Molnar A, Gellynck X (2013) Food quality management system: reviewing assessment strategies and a feasibility study for European food small and medium-sized enterprises. *Food Control* 31:607–616
- Duda RO, Hart PE, Stork DG (2001) Pattern classification. Wiley, New York
- Franke K, Tschuschner HD (1991) Modelling of the continuous high shear rate conching process for chocolate. *J Food Eng* 14:103–115
- García-Muñoz S, Kourti T, MacGregor JF, Mateos AG, Murphy G (2003) Troubleshooting of an industrial batch process using multivariate methods. *Ind Eng Chem Res* 42:3592–3601
- Glicerina V, Balestra F, Dalla Rosa M, Romani S (2013) Rheological, textural and calorimetric modifications of dark chocolate during process. *J Food Eng* 119:173–179
- Glicerina V, Balestra F, Dalla Rosa M, Romani S (2015) Effect of manufacturing process on the microstructural and rheological properties of milk chocolate. *J Food Eng* 145:45–50
- González-Martínez JM, Ferrer A, Westerhuis JÁ (2011) Real-time synchronization of batch trajectories for on-line multivariate statistical process control using dynamic time warping. *Chemom Intell Lab Syst* 105:195–206
- Jackson JE, Mudholkar GS (1979) Control procedures for residuals associated with principal component analysis. *Technometrics* 21(3):341–349
- Kassidas A, MacGregor JF, Taylor PA (1998) Synchronization of batch trajectories using dynamic time warping. *AIChE J* 44(4):864–875
- Kourti T (2003a) Multivariate dynamic data modeling for analysis and statistical process control of batch processes, start-ups and grade transitions. *J Chemom* 17:93–109
- Kourti T (2003b) Abnormal situation detection, three-way data and projection methods; robust data archiving and modeling for industrial applications. *Ann Rev Control* 27:131–139

- Kourti T, MacGregor JF (1996) Multivariate SPC methods for process and product monitoring. *J Qual Technol* 28:409–428
- Kuang TH, Yan Z, Yao Y (2015) Multivariate fault isolation via variable selection in discriminant analysis. *J Process Control* 35:30–40
- Lim SAH, Antony J, Albliwi S (2014) Statistical process control (SPC) in the food industry—a systematic review and future research agenda. *Trends Food Sci Technol* 37:137–151
- Lu N, Gao F, Yang Y, Wang F (2004) PCA-based modelling and on-line monitoring strategy for uneven-length batch processes. *Ind Eng Chem Res* 43:3343–3352
- MacGregor JF (1997) Using on-line process data to improve quality: challenges for statisticians. *Int Stat Rev* 65:309–323
- Nomikos P, MacGregor JF (1994) Monitoring batch processes using multiway principal component analysis. *AIChE J* 40(8):1361–1375
- Nomikos P, MacGregor JF (1995) Multivariate SPC charts for monitoring batch processes. *Technometrics* 37(1):41–59
- Owusu M, Petersen MA, Heimdal H (2012) Effect of fermentation method, roasting and conching conditions on the aroma volatiles of dark chocolate. *J Food Process Preserv* 36:446–456
- Prawira M, Barringer SA (2009) Effects of conching time and ingredients on preference of milk chocolate. *J Food Process Preserv* 33:571–589
- Ramaker HJ, Van Sprang ENM, Westerhuis JA, Smilde AK (2003) Dynamic time warping of spectroscopic batch data. *Anal Chim Acta* 498:133–153
- Torres-Moreno M, Tarrega A, Costell E, Blanch C (2012) Dark chocolate acceptability: influence of cocoa origin and processing conditions. *J Sci Food Agric* 92:404–411
- Woodall W, Montgomery D (2014) Some current directions in the theory and application of statistical process monitoring. *J Qual Technol* 46:78–94

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