Preprints of the 19th World Congress
The International Federation of Automatic Control
Cape Town, South Africa. August 24-29, 2014

Product Quality Estimation Using Multivariate Image Analysis ⋆

John Loftus * **David Laurí** ** **Barry Lennox** ***

* *The University of Manchester, Control Systems Centre (e-mail: john.loftus@postgrad.manchester.ac.uk).*
** *Advanced Manufacturing Technology Group, Pfizer Inc, Peapack, New Jersey, USA (e-mail: David.LauriPla@pfizer.com).*
*** *The University of Manchester, Control Systems Centre (e-mail: barry.lennox@manchester.ac.uk).*

Abstract: This paper presents a novel method for estimating the quality of products from a proprietary process using Multivariate Image Analysis. The ability to estimate product quality would be useful for identifying production steps that are potentially problematic and would also help to reduce waste by ensuring that any defective products are detected before they undergo any further processing. The proposed method extracts textural and spectral features from images of products classified as either 'good' or 'bad'. These features are then combined to form two data matrices, one for good products and one for bad products, which are then used for subsequent analysis. After pre-processing, Principal Component Analysis is used to produce quality models for both grades of product. Data from bad products are projected onto the model for good products and vice versa. Statistical measures, specifically the Square Prediction Error and leverage, are then used to classify the quality of new products. Results suggest that using the proposed methodology can aid in the estimation of product quality, although further work must be undertaken to provide a more critical analysis of the proposed technique.

Keywords: Automatic recognition; Image analysis; Industrial production systems; Industry automation; Manufacturing processes; Multivariate quality control; Pattern recognition;

1. INTRODUCTION

Modern industrial processes are increasingly required to reduce operating costs and process downtime, whilst improving efficiency and product quality. Consequently, more advanced monitoring and control strategies are required. Due to the inherent complexity of modern industrial processes, product quality can be difficult or impractical to measure on-line. Increasingly, visual inspection of products is being used as a means of assessing overall product quality and due to modern advances in imaging hardware and analysis tools, on-line imaging systems offer an attractive alternative to off-line systems. There are a number of areas in which image analysis can be beneficial to industrial processes. For example, imaging systems can be used to identify defective products and to classify and quantify products accordingly. They may also be used to estimate overall product quality, monitor process conditions and provide data for control purposes [Duchesne et al., 2012]. However, one of the main difficulties of image analysis lies in the efficient extraction of useful information from the images themselves [Bharati, 2002].

The work described in this paper focuses upon the use of Multivariate Image Analysis (MIA) to measure the quality of products from a proprietary process. MIA is a technique that was first proposed by Geladi et al. [1989] and Esbensen and Geladi [1989] in the late 1980's and essentially involves applying multivariate statistical methods, for example Principal Component Analysis (PCA), to a multivariate image. A multivariate image is defined as an image consisting of multiple spectral bands. Such an image consists of a stack of congruent images, with each image corresponding to a different wavelength. Alternatively, a multivariate image can be thought of as a two-way array of pixel intensity vectors, with a single vector at each pixel location [MacGregor et al., 2001].

A general framework for image analysis was proposed by Liu [2005] and involves a series of steps, which are shown in figure 1. The work reported here concentrates on the final two stages of this framework, namely the feature extraction and feature analysis stages.

1.1 Related Works

Early works were centred on the use of MIA to analyse multivariate images taken from subjects such as medical imaging [Geladi and Grahn, 1996], remote sensing [Esbensen and Geladi, 1989] and analytical chemistry [Geladi and Esbensen, 1989, Geladi and Grahn, 1996]. MacGregor et al. [2001] then proposed that MIA could be used for on-line industrial process monitoring by applying the method to a time series of images. The concepts introduced by these authors were first applied to an industrial softwood lumber process for on-line grading purposes [Bharati and

⋆ This work was supported in part by the Engineering and Physical Sciences Research Council (EPSRC), through a Doctoral Training Award (DTA).

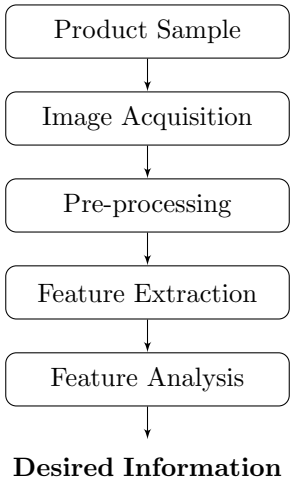


Fig. 1. Framework for MIA. Adapted from [Liu, 2005].

MacGregor, 2003]. Yu and MacGregor [2003] then used MIA for on-line monitoring of snack food coatings.

The approach to MIA proposed in this paper is different from other approaches in two ways. The first difference is in the identification of textural features from an image, which are then subsequently used to construct a regression matrix. Current textural analysis methods can be divided into four main categories, which are structural, model-based, statistical and transform-based methods. Structural methods describe textural features using simple texture elements and spatial arrangement rules. However, these methods are limited by the fact that they can only describe regular textures. Statistical methods are widely used and textural features are represented by analysing the gray level properties of an image. Both structural and statistical methods are covered in more detail in Haralick [1979]. Model-based methods use parameter estimation techniques to determine an empirical texture model, but these methods can be computationally intensive and complex to implement [Materka and Strzelecki, 1998]. Finally, transform based methods, including Fourier and wavelet transforms represent the state of the art, but these methods can be more complex to implement and evaluate. A review of texture analysis methods is provided by Bharati et al. [2004]. The methodology described in this paper is related to statistical methods, but the approach differs in that the textural features are extracted by comparing each individual pixel to its nearest one neighbour, which is a simpler approach than other statistical methods. The second difference is in the techniques used to estimate product quality from the initial data matrix. The quality models reported here are constructed using PCA and associated statistics, which is contrary to many other reported techniques, which use regression methods, such as Partial Least Squares (PLS), to estimate product quality.

The paper is organised as follows: Section 2 details the multivariate data analysis techniques inherent to the proposed technique, including PCA, Square Prediction Error (SPE) and leverage. Section 3 describes the case study and the methodology employed. Section 4 presents the results of the case study and finally section 5 presents the conclusions.

2. MATHEMATICAL PRELIMINARIES

2.1 Principal Component Analysis

PCA is a prevalent multivariate data analysis technique that has been used successfully in a wide range of applications and a large amount of literature exists that pertains to this subject including Mardia et al. [1979], Wold et al. [1987] and Jackson [1991].

As previously described, MIA effectively applies multivariate statistics, in this case PCA, to an image, which can be thought of as a source of multivariate data. It is therefore appropriate to describe the PCA method. PCA involves decomposing a data matrix X into structure and noise components and allows large datasets to be represented in a lower dimensional subspace, with the dimensionality of the subspace being determined by the number, A, of principal components used in the model. The PCA technique is defined by (1).

$$X = \sum_{a=1}^{A} t_a p_a^T + E \tag{1}$$

Where:

$$\begin{aligned} X &= \text{Original data matrix} \\ t_a &= \text{Score vector for } a^{th} \text{ component} \\ p_a &= \text{Loading vector for } a^{th} \text{ component} \\ E &= \text{Residual matrix} \\ A &= \text{Number of principal components} \end{aligned}$$

The starting point for PCA is a data matrix X. In the case of MIA, the X matrix represents an individual image and contains a two dimensional array of pixel intensity vectors, with one vector at each pixel location in the image [MacGregor et al., 2001]. The first principal component explains the greatest amount of variance in the original data matrix. The second principal component explains the second greatest variance and so forth until all the variance has been accounted for. A key aspect of PCA is determining the optimal number of components to use for analysis. To determine the optimal number of components required to adequately describe the data structure, methods including cross-validation techniques can be used. The insignificant components can then be discarded and the dimensionality of the original data matrix reduced. The reader is referred to Wold et al. [1987] for a more comprehensive description of PCA.

2.2 Squared Prediction Error

The Squared Prediction Error (SPE) is calculated from the rejected PCA scores and represents the information in the original matrix that is not explained by the PCA model.

The SPE of an object, n, is equal to the sum of the square of the discarded scores and is defined by (2).

$$SPE_i = \sum_{i=A+1}^{K} t_i t_i^T \tag{2}$$

Alternatively, SPE can be calculated directly from the residual matrix, E, using (3).

$$SPE_i = e_i e_i^T \tag{3}$$

2.3 Leverage

Leverage is a measure of the effect that an object has on the multivariate model and is to some extent related to the distance of that particular object from the model centre. Leverage values for individual objects are scaled such that values are between zero and one. Objects that have high leverage have a greater effect on the model, are further away from the model centre and have values closer to one. Objects with low leverage have less effect on the model, are closer to the model centre and have values close to zero [Esbensen et al., 2002]. Leverage is calculated using equation (4).

$$h_i = \frac{1}{n} + \sum_{a=1}^{A} \frac{t_{ia}^2}{t_a^T t_a} \tag{4}$$

Where:

h_i = Leverage for object i
t_{ia} = Score for object i in the a^{th} component
A = Number of principal components
n = Total number of objects

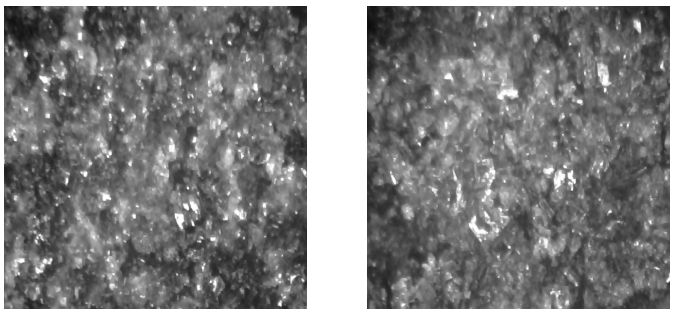
3. CASE STUDY

3.1 Decafé 'Alika' Production

The aim of the proposed technique was to grade the quality of Decafé products. Decafé is a patented material from Raúl Laurí Design Lab [Laurí, 2013] that is used to create a wide range of products. The Decafé production process is not fully described due to proprietary reasons, but the concept is as follows: Decafé production consists of mixing used coffee grounds with a natural binding substance, which then undergoes further pressure and temperature based transformation.

This particular case study involves grading the quality of 'Alika' bowls from microscope images. 'Alika' is a bowl made from the Decafé product. There are two groups of images, which correspond to good and bad products. Bad products are those that show cracks on the surface. The ultimate aim is to use MIA to construct two models that can then be used to systematically quantify the quality of a particular bowl given the microscope images.

Images are acquired from both 'good' and 'bad' products, examples of which are shown in figure 2. The image on the left represents a good product, while the image on the right represents a bad product. Each individual image contains 1600 × 1200 pixels. In addition, each image covers 7mm^2 of each product, with each product measuring 23cm in diameter. It is very difficult, if not impossible, to visually distinguish between good and bad products from the partial images in regions in which the cracks do not show. Therefore, a model that would enable the classification of products based on images would be beneficial in detecting defective products before they undergo any further processing.



(a) Image of Good Product (b) Image of Bad Product

Fig. 2. Example images: Good (a) and Bad (b) products.

3.2 Methodology

The proposed methodology for estimating the quality of 'Alika' bowls is described in the following sequence of steps and is illustrated in figure 3. The described methodology uses 10% of each image for analysis, but it should be noted that the results reported here are similar to results obtained using between 5% and 25% of each image, which indicates that the chosen technique is robust. A final value of 10% of each image for analysis was chosen to reduce computational intensity, whilst maintaining good separation between product classes.

Feature Extraction For each image, 10% of the pixels along the central y-axis were used for analysis, which is equal to 1600 × 120 pixels. From this 10%, both textural and spectral features were then extracted. To extract textural features, the pixels were firstly converted from RGB to grayscale. For each individual pixel of the grayscale image, three characteristics of the nearest one neighbour to that pixel were evaluated. These characteristics were the maximum, mean and standard deviation differences. Using the same 10% of the image, spectral features are extracted using Red, Green and Blue (RGB) channels. Each individual pixel is therefore described by six numerical values. The 2D matrices of features for each of the 50 images are then combined into a 3D data matrix, $\underline{X}$, which has dimensions $(I \times J \times K)$, where I is the number of images, J is the total number of pixels of the subimage and K is the number of pixel features. $\underline{X}$ was then unfolded using batch-wise unfolding. The resulting 2D matrix has dimensions $(I \times JK)$, is 'short and fat' and contains a large amount of redundant information, which is similar to spectral data.

Model Development The dataset used for analysis consisted of 50 images in total; 20 representing good products and 30 representing bad products. Five images were taken for each product, therefore the 50 images used in the analysis only represented ten products in total, four good products and six bad products. In subsequent figures, the good products are labelled A to D, with subscripts 1-5 denoting the specific image for that product. Similarly, bad products are labelled E-J and subscripts 1-5 denote the specific image for that product.

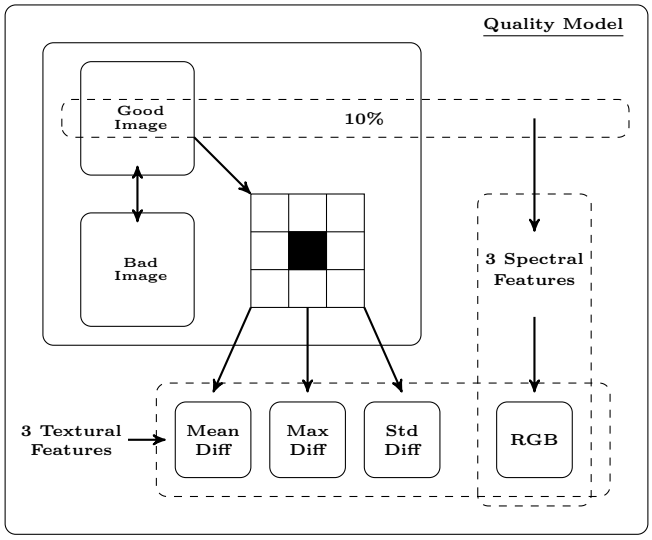


Fig. 3. Methodology used to construct X matrix

After autoscaling, the matrix of textural and spectral features, X, was divided into good and bad datasets, each of which was further divided into calibration and validation datasets. To develop the model for good products, 15 'good' images were used for model calibration and the remaining 35 images used for validation. For the bad product model, 20 'bad' images were used for calibration and the remaining 30 for validation. The individual products used for calibration and validation were chosen at random. It was hypothesised that the leverage values for the bad data, when projected onto the good model (and vice versa), would provide separation between the two classes, since the projected data would lie far from the model centre and would have larger SPE values. To test this hypothesis, two PCA models were constructed, one for good products and one for bad products. Data from 'bad' images were then projected onto the good model and data from 'good' images were projected onto the bad model. The level of separation between products for both models was then evaluated using leverage and SPE.

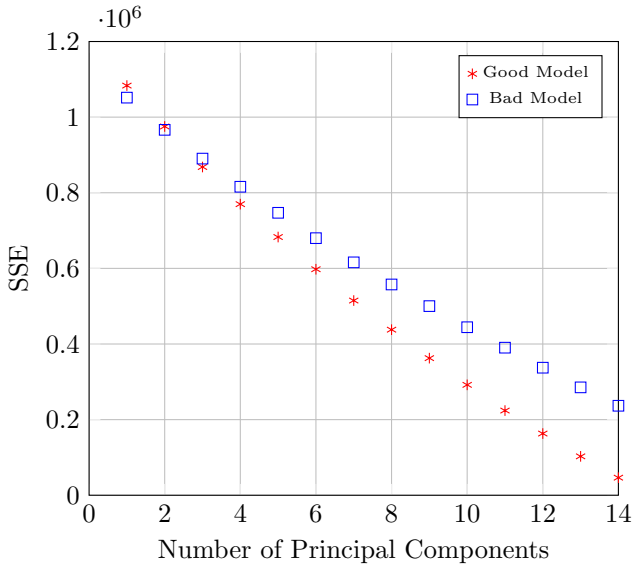


Fig. 4. Principal Component Selection

To develop PCA models, it was firstly necessary to determine the optimal number of components to be used in each model. This was done by evaluating the Sum Square Error (SSE) versus number of principal components, the results of which are shown in figure 4. Wise and Gallagher [1996] suggest using the number of principal components that corresponds to a 'knee point' in the graph, but it is evident from figure 4 that there is no such point for either model. It should be noted that cross-validation techniques can also be used to determine an optimal number of components, but this method was not used as it was found to be computationally inefficient and results were difficult to obtain in a timely fashion. The optimal number of components for each model was therefore determined using the cumulative variance captured. Cumulative variance values in excess of 50% for both models were deemed to be sufficient for model development. This value was chosen to optmise the level of separation between product classes. The results of the percentage variance captured for each model are shown in table 1. PCA models were developed using between 6-10 components and the amount of separation between product classes was evaluated. The results reported in the following section are for 8 and 10 principal components respectively, since use of these numbers of components achieves a balance between product separation and model accuracy. Figure 4 also shows that the SSE is larger for the model for bad products than the good products and for the same number of principal components, the good model explains more variance than the bad model, which is further verified by table 1. Therefore, it is expected that the SPE values will be larger for the bad model than for the good one.

Number of PC's	**% Variance Captured (Cumulative)**	
	Good Model	Bad Model
4	36.64	28.71
6	50.80	40.59
8	63.96	51.29
10	75.97	61.17

4. RESULTS

Having chosen an appropriate number of principal components, PCA models were developed for both good and bad products. Figures 5 and 6 show the results for both good and bad models using 8 principal components and figures 7 and 8 show the results of models developed using 10 principal components. By comparing the calibration data for both models it is evident that as the number of principal components increases from 8 to 10, the separation between product classes increases. For both 8 and 10 principal components, the separation between classes is more pronounced in the good model, which can be attributed to the fact that the good model captures more variance than the bad model, as seen in figure 4 and table 1. On the whole, the good model seems to out-perform the bad model from a separation perspective. There is an increase in the separation of calibration data for both models as the number of principal components increases from 8 to 10. As a general rule, as the number of PCs increases, the amount of separation between products increases and this is mainly due to the SPE increasing. However, as more components are used, the models are prone to over-fitting

the calibration data, which can lead to unreliable results and artificial separation between product classes.

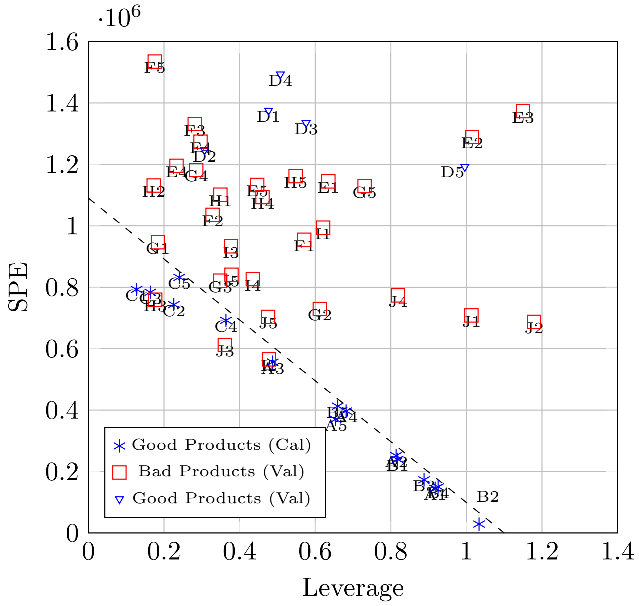


Fig. 5. Leverage vs. SPE for 8 PCs - Good Model. Class separation by SPE $= 1.09 \cdot 10^6(\text{Lev}) + 1.199 \cdot 10^6$

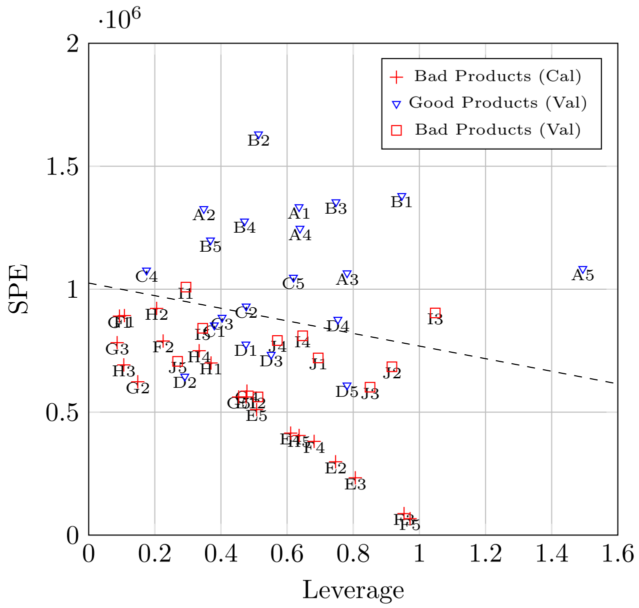


Fig. 6. Leverage vs. SPE for 8 PCs - Bad Model. Class separation by SPE $= 256.3 \cdot 10^3(\text{Lev}) + 10.25 \cdot 10^5$

Although the results from the calibration data suggest that there is some separation between classes, the validation data is not consistent with this. Examination of figures 5 to 8 reveal that the validation data, namely products I and J, for bad products is broadly consistent with the calibration data in both good and bad models. However, the validation data for good products (product D) is problematic since the PCA method fails to classify the product correctly in both good and bad models. For both 8 and 10 components, all product D images are classified as a bad product rather than a good one, which is contrary to what is expected. However, in the next stage of the

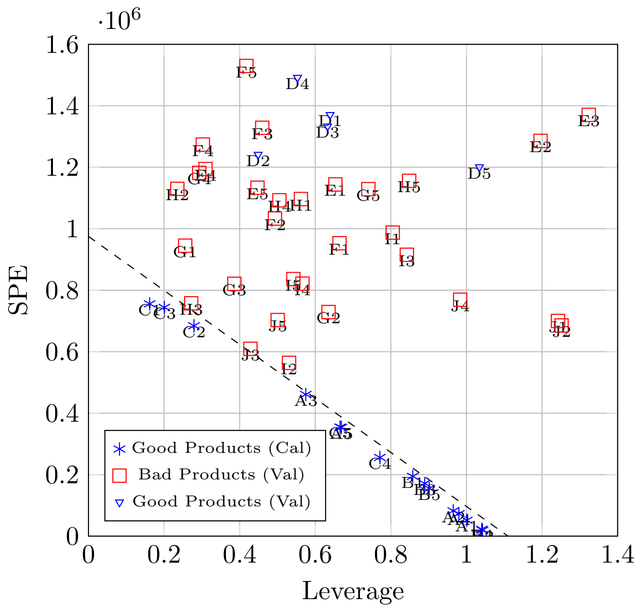


Fig. 7. Leverage vs. SPE for 10 PCs - Good Model. Class separation by SPE $= 8.86 \cdot 10^5(\text{Lev}) + 9.75 \cdot 10^5$

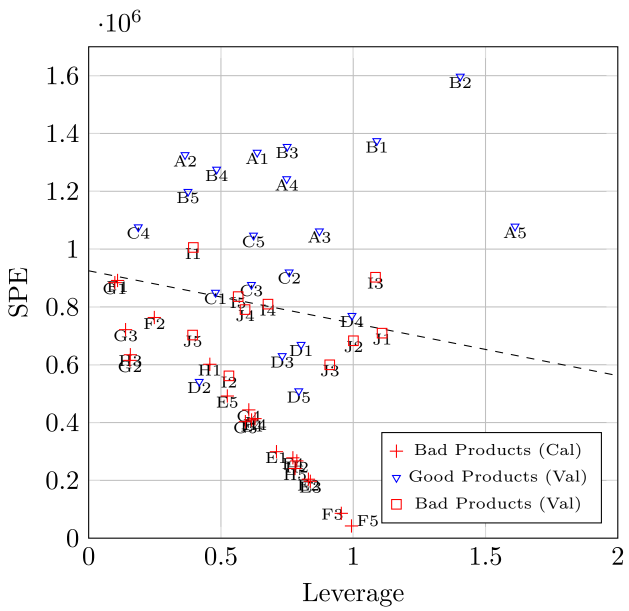


Fig. 8. Leverage vs. SPE for 10 PCs - Bad Model. Class separation by SPE $= 181.37 \cdot 10^3(\text{Lev}) + 9.25 \cdot 10^5$

production process, product D started to show some small cracks, which means that product D was actually a bad product, even though it did not show cracks at the end of the first phase of the production process, which is when the microscope images were taken. With this in mind, it can be seen that the product images used for validation have actually been classified correctly, which indicates that the models were able to classify a bad product even before cracks were visible in the product.

Having developed PCA models for both classes of product, simple linear classifiers can now be derived for both good and bad products. These linear classifiers are depicted in figures 5 to 8 and have been derived using the linear least squares method. The success of these classification

rules are summarised in table 2. From these results, it can be seen that for both 8 and 10 PCs, the good model outperforms the bad model. Also, when using 10 PC's, the good model achieves a 100% success rate across both calibration and validation datasets. Table 2 also shows that the good model outperforms the bad model, with the good model achieving a 100% success rate for both 8 and 10 principal components. This is believed to be due to the fact that the good model captures more variance than the bad model for the same number of principal components. It should be specified that these results are preliminary, and the performance of this technique should be further assessed on a larger set of products.

PC's	**Classification Statistics - Validation**			
	Good Model		Bad Model	
	Val - Good	Val - Bad	Val - Good	Val - Bad
8	100%	90%	70%	80%
10	100%	100%	80%	60%

5. CONCLUSIONS

This paper has investigated the use of principal component analysis and associated statistics, specifically square prediction error and leverage, for estimating the quality of products from a proprietary process. Related bodies of work have been discussed and mathematical prerequisites have been described. The particular case study has then been outlined and the proposed methodology for estimating product quality using PCA, SPE and leverage has been discussed.

The key stages of the described methodology are as follows: Firstly, textural and spectral features are extracted from a section of each image representing good and bad products. These features comprise the data matrix from which two PCA models are calibrated, one for good products and one for bad products. Bad product data is then projected onto the good model and good product data is projected onto the bad model. The subsequent leverage versus SPE plots have then been used to estimate product quality. Model validation suggests that the proposed methodology has some merit and could be used to provide a preliminary estimate of product quality for the described process. A simple linear classifier has been proposed for each model and the good model has successfully classified all validation data correctly. The results also show that the good model performs better than the model for bad products. The models developed could potentially be used to provide an on-line estimate of product quality and would enable products estimated as bad to be examined in more detail or removed from further downstream processing.

ACKNOWLEDGEMENTS

This work was supported in part by the Engineering and Physical Sciences Research Council (EPSCR) through a Doctoral Training Award (DTA). The authors would like to thank Mr. Raúl Laurí for providing the original product images and process information. The author has also been supported by Academic Partnership Funding from Advanced Manufacturing Technology Group, Pfizer Global Supply, to promote academic research in Intelligence based Biopharmaceutical Manufacturing.

REFERENCES

M. H. Bharati. *Multivariate image analysis and regression for industrial process monitoring and product quality control*. Ph.D. thesis, McMaster University, Canada, 2002.

M. H. Bharati, J. J. Liu and J. F. MacGregor. Image texture analysis: methods and comparisons. *Chemometrics and Intelligent Laboratory Systems*, 72:57–71, June 2004.

M. H. Bharati and J. F. MacGregor. Softwood lumber grading through on-line multivariate image analysis techniques. *Industrial & Engineering Chemistry Research*, pages 5345–5353, 2003.

C. Duchesne, J. J. Liu, and J. F. MacGregor. Multivariate image analysis in the process industries: A review. *Chemometrics and Intelligent Laboratory Systems*, 117: 116–128, Aug 2012.

K. Esbensen and P. Geladi. Strategy of multivariate image analysis (MIA). *Chemometrics and Intelligent Laboratory Systems*, 7(1-2):67–86, Dec 1989.

K. Esbensen, D. Guyot, F. Westad, and L.P. Houmoller. *Multivariate Data Analysis - in practice: An introduction to multivariate data analysis and experimental design*. CAMO, 2002.

P. Geladi and K. Esbensen. Can image analysis provide information useful in chemistry? *Journal of Chemometrics*, 3(2):419–429, 1989.

P. Geladi and H. Grahn. *Multivariate Image Analysis*. Wiley, 1996.

P. Geladi, H. Isaksson, L. Lindqvist, S. Wold, and K. Esbensen. Principal component analysis of multivariate images. *Chemometrics and Intelligent Laboratory Systems*, 5(3):209–220, Mar 1989.

R. M. Haralick. Statistical and structural approaches to texture. *Proceedings of the IEEE*, 67(5):786–804, 1979.

J. E. Jackson. *A User's Guide to Principal Components*. A Wiley-Interscience publication. Wiley, 1991.

R. Laurí. Raúl Laurí Design Lab. ONLINE. Available at www.rlauri.com, 2013.

J. Liu. *Machine vision for process industries: monitoring, control, and optimization of visual quality of processes and products*. Ph.D. thesis, McMaster University, Canada, 2005.

J. F. MacGregor, M. H. Bharati, and H. Yu. Multivariate image analysis for process monitoring and control. *Process Imaging for Automatic Control*, (17), 2001.

K. V. Mardia, J. T. Kent and J. M. Bibby. *Multivariate analysis*. Probability and mathematical statistics. Academic Press, 1979.

S. Materka and K. Strzelecki. Texture analysis methods - A review. *Technical University of Lodz, Institute of Electronics, COST B11 Report*. Brussels, 1998.

B. M. Wise and N. B. Gallagher. The process chemometrics approach to process monitoring and fault detection. *Journal of Process Control*, 6(6):329–348, Dec 1996.

S. Wold, K. Esbensen and P. Geladi. Principal component analysis. *Chemometrics and Intelligent Laboratory Systems*, 2:37–52, Aug 1987.

H. Yu and J. F. MacGregor. Multivariate image analysis and regression for prediction of coating content and distribution in the production of snack foods. *Chemometrics and Intelligent Laboratory Systems*, 67(2):125–144, Aug 2003.