INFLUENCE OF FOOD BY-PRODUCTS ADDITION ON THE SPECTRAL CHARACTERISTICS OF BAKERY PRODUCTS

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Abstract**:** The work in this paper is aimed to determine the impact of the added by-products on spectral characteristics of bakery products. Cookies with added apple skin powder and cakes with grape pomace powder are analyzed. Three methods for data reduction of spectral characteristics are used: latent variables, linear and non-linear variant of principal components. The selection of data reduction method is based on Naïve Bayesian classifier. Data from the selected non-linear variant of principal components are used for classification with discriminant analysis and support vector machines methods. The results of the separation of object areas of bakery products strongly depend on the method of features extraction and reducing the input data, as well as on the method of classification. Better results are obtained with non-linear variant of support vector machines method, in comparison with its linear variant and discriminant analysis.

Keywords**:** cookies, sponge cakes, by-products, spectral characteristics, data reduction, classification

1. Introduction

The food industry produces large quantities of waste each year, and their efficient management and use is one of the basic goals of the European Union [6,8,15]. This type of waste is a source of: fibers, proteins, carbohydrates, aromatic compounds, etc. [14].

Apple skin powder (ASP) is a secondary product that is obtained after the production of canned apples, dried apples, the production of apple puree and apple pie [19].

Grape pomace powder (GPP) is the solid residue generated by the wine industry and accounts for about 20-30% of the total weight of the grapes. GPP is most frequently used as animal feed or as compost. The chemical composition of GPP depends on the type of grapes, the location of the wine plantations, the agricultural mechanical conditions during the growing of the grapes as well as the conditions during the wine production [16].

Known methods and technical tools for evaluating changes in the quality of bread products [4,5,20] show that systems for obtaining, processing and analyzing spectral characteristics find application in the field of study. They achieve good accuracy in the classification of external or internal characteristics, and the cost of technical implementation of the systems working with them is significantly lower compared to hyperspectral images. Methods related to spectral analysis are preferable to methods based on digital images and colorimeter measurements, as they can provide information on both the surface texture and the internal structure of products depending on their composition [2,11].

In the spectral analysis method, one of the main advantages is that it is easy to use and suitable for detecting internal defects in food. A disadvantage of the direct use of spectral characteristics is their limited sensitivity to small changes in object properties. In the case of minor changes in the composition of the product, methods to reduce the volume of spectral characteristics data are appropriate. They provide a new character space and speed up the computational process [17].

The aim of this paper is to determine the impact of the added by-products (ASP and GPP) on spectral characteristics of baked goods

2. Material and methods

The used raw materials for the production of cookies and sponge cakes are purchased from the local shops in Razgrad, Bulgaria. The cookies were produced according to the AACC 10-50D method [1] with some modifications, and the sponge cake was produced according to the method presented by Velioğlu et al., 2017 [18] with some modifications.. If was produced six types of cookies (control - 100% wheat white flour and (4%, 8%, 16%, 24% and 32%) of apple skin powder (ASP)) and five types of sponge cakes (control - 100% wheat white flour and sponge cakes with 4%, 6%, 8% and 10% grape pomace powder (GPP)).

The nomenclature used is:

P1-100%Wheat; P2-4%ASP; P3-8%ASP; P4-16%ASP; P5-24%ASP; P6-32%ASP.

C1-100%wheat; C2-4%GPP; C3-6%GPP; C4-8%GPP; C5-10%GPP.

Figure 1 presents the cookies with apple skin powder.

P1 P2 P3 P4 P5 P6

Figure 1. Cookies with apple skin powder – general view

Figure 2 presents the sponge cakes in general view.

C1 C2 C3 C4 C5

Figure 2. Sponge cakes with grape pomace powder – general view

The obtaining of **spectral characteristics** was done by converting LMS model values into reflectance spectra in the VIS range, in the range 390-730nm, by mathematical dependencies where conversion is possible in both directions of equality [9]. The conversion functions applied are 10° observer (Stiles and Burch 10°, RGB (1959)) and illumination D65 (average daylight with UV component (6500K)).

Latent variables **(LV)** obtained by partial least squares regression (PLSR) [12]. PLS (Partial least-squares) regression is a technique used for data that contains correlated predictive variables. This technique constructs new predictive variables known as components as a linear combination of the original predictive values. PLS constructs these components by assuming the observed values, resulting in a more accurate model with better forecasting.

In the principal components analysis **(PCA)** [13,17], the extraction of characteristic properties is a transformation of the original data with all of its variables into a sample of reduced ones. All measurements or variables that are designed in a small size area are used. The principal component analysis (PCA) creates an orthogonal coordinate system where the axes are arranged according to the dispersion in the original data to which the corresponding major component and the dispersions and the principal values are related.

The Kernel variant of PCA **(kPCA)** [10] is an expansion of the PCA using kernel techniques. Using a single kernel, the original kPCA transformation takes place in a new space of high dimension (reproduction kernel Hilbert space) with non-linear mapping of the input data. The kernel K in this work is defined by K(x,y)=-exp((x-y)^2/(sigma)^2), where sigma is setting parameter.

Naïve Bayes classifier **(NBC)** [3] is one of the classical algorithms in machine learning, which is based on the Bayes theorem for determining the apisterior probability of an event occurring. Assuming the "naïve" assumption of conditional independence between each pair of features. The purpose of the classification is to determine the class to which the object x belongs. Therefore, it is necessary to find a probabilistic class of object x, ie. it is necessary for all classes to choose the one that gives the maximum probability P(y=c|x).

The discriminant function analysis **(DA)** [12] used is a multidimensional data analysis that is applied when there is a need to "predict" the values of a clustering variable. This is also called classification or image recognition. Linear discriminant analysis constructs linear discriminative functions from predictors. The goal is to obtain a rule for assigning a new observation to a class. Assigning or "allocating" to a certain class of characteristics is also necessary for the present development. The following separation functions are used in the discriminative analysis:

Linear **(L)** - Regularized linear discriminant analysis (LDA). All classes have the same covariance matrix;

DiagLinear **(DL)** – Same as linear, but all classes have the same, diagonal covariance matrix;

Quadratic **(Q)** - a quadratic discriminant function (second degree), distributes multivariate normal density data by calculation of covariance and collects them in a group;

DiagQuadratic **(DQ)** - similar to the quadratic separating function, but uses the calculation of a covariance matrix diagonal (diagonal non-linear separating function);

Mahalanobis **(M)** - divides the data into groups by distance from Mahalonobis defining covariance in the data.

The other classifier used is the support vector machines **(SVM)** method [7], which is a model with teacher training and related algorithms for data analysis used for classification. In a learner, each element is associated with one of two categories, and the trainer algorithm builds a model in which the data is transformed into a new space. The created model represents the data in the new space so that there is separation between them. The SVM analysis method used, has the following kernel separation functions:

Linear kernel **(L)** - default for two-class learning;

Quadratic **(Q)** - a quadratic separating function (second degree), distributes multivariate normal density data by calculation of covariance and collects them in a group;

Polinomial **(Poly)** - polynomial separating function;

RBF - a separation function defined by radial basis elements.

The evaluation of the performance of the classifiers used is based on a general classification error, which is described by the formula:

$$\mathrm{e} = \frac{\sum_{i=1}^{n}\left(\sum_{k=1}^{n} y_{ik} - y_{ii}\right)}{\sum_{i=1}^{n}\sum_{k=1}^{n} y_{ik}}.100,\% \qquad (1)$$

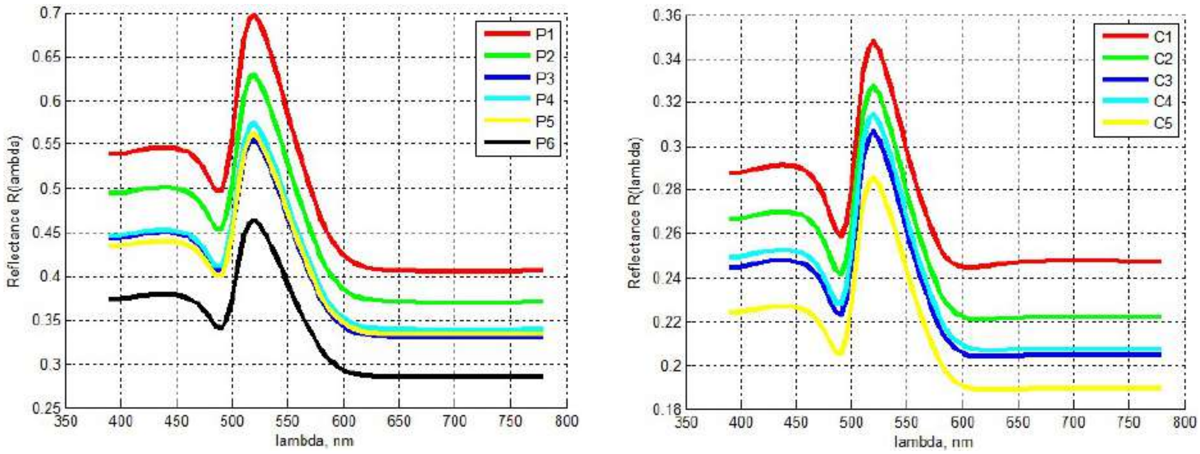
where y_{ik} is the number of class i samples classified by classifier in class k; yii - number of correctly recognized samples; k = 1... n - number incorrectly assigned to a class i relative to the total number of samples; n - number of classes.

All calculations are made at a level of significance α=0,05.

3. Results and discussion

Spectral characteristics of cookies and cakes with the addition of food by-products are obtained. The spectral characteristics data are reduced with latent variables and principal components. The data separability for the tested products is estimated, depending on their composition. For this purpose, the methods of classification discriminant analysis and the method of support vector machines, with a total of 9 linear and nonlinear separating functions, were used. An analysis of the obtained results is made.

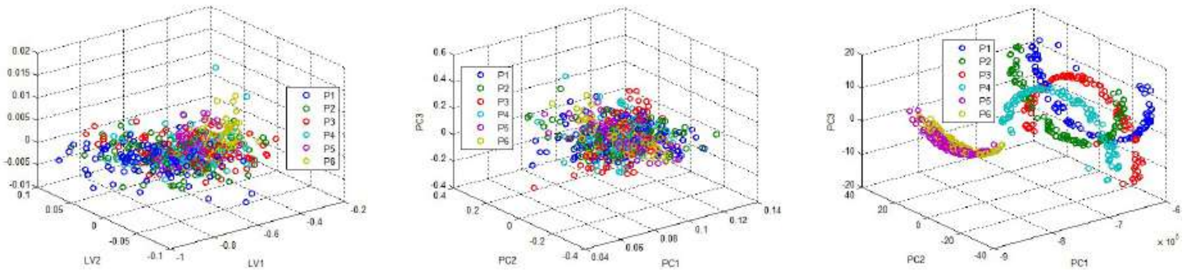
The obtained spectral characteristics of cookies and cakes with additives are shown in average on figure 3. All spectral characteristics obtained are not suitable for visualization because of their strong overlap. It is necessary to analyze the separation of the products, depending on the amount of ASP and GPP added, by methods of reducing the amount of data from the spectral characteristics.



a) Cookies ASP b) Cakes GPP

Figure 3. Spectral characteristics of cookies and cakes

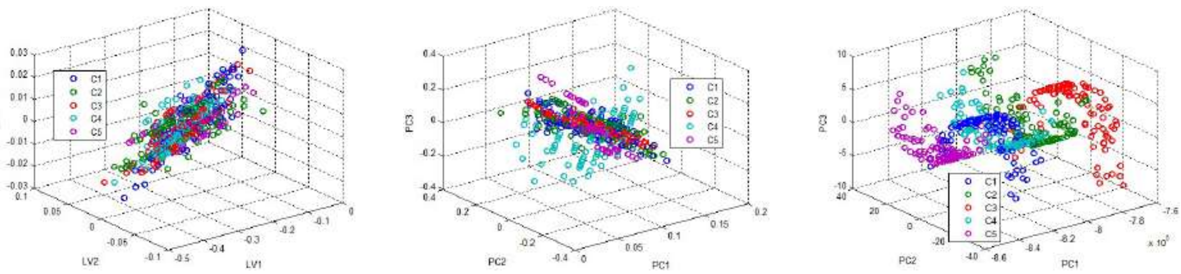
Figure 4 shows the results of reducing the amount of data on the spectral characteristics of cookies by three methods. It can be seen that using latent variables and a linear variant of the principal components results in overlapping of the data for different types of cookies. When using a kernel variant of the principal components, a non-linear kernel shows the apparent separability of the data for the different cookies, depending on their composition. This separability needs to be verified through classifiers.



a) LV b) PC c) kPC

Figure 4. Reduced spectral response data for cookies

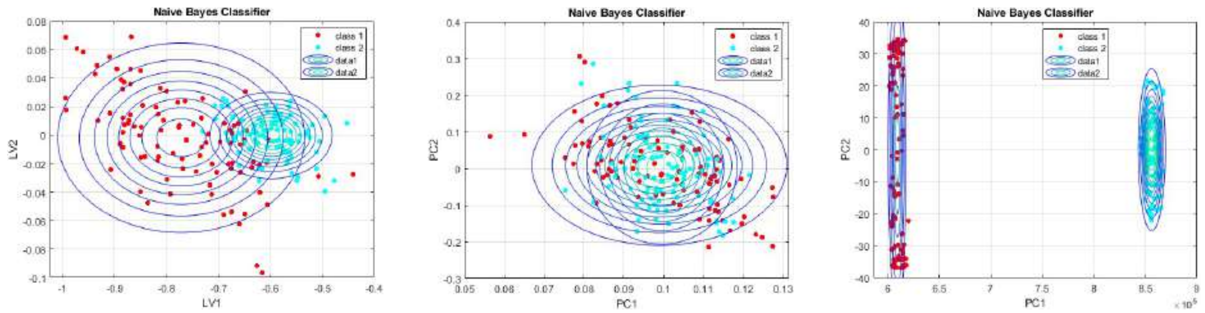
Figure 5 shows the results of reducing the amount of data of spectral characteristics of cakes by three methods. As with the previous product, the use of latent variables and principal components is not appropriate here. The principal components with non-linear kernel function are suitable. They have a visible separation of the cakes, depending on the amount of GPP.



a) LV b) PC c) kPC

Figure 5. Reduced data from spectral characteristics for cakes

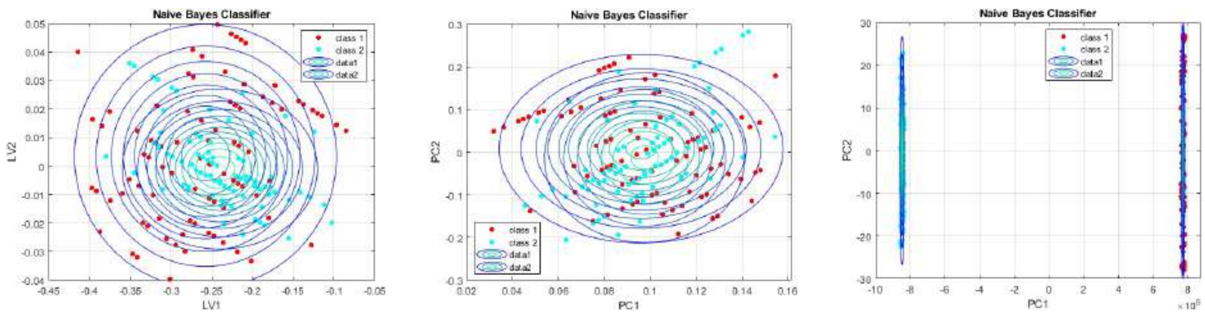
The Naïve bayes classifier was used as the base class due to the fact that part of the data classes overlapped. Figure 6 shows examples of classification with a Naïve Bayes classifier using reduced cookies spectral data. The observed overlap of experimental data also influences the classification. When using latent variables and the linear variant of principal components, the values of the general classification error are significantly greater than 10%. The problem is a solution to the use of a non-linear kernel in reducing the amount of spectral data. In this case, a zero classification error is observed.



a) LV, e=14% b) PC, e=37% c) kPC, e=0%

Figure 6. Classification with Naive Bayes Classifier for Cookies P1-P5

Figure 7 shows examples of classification with a Naive Bayes classifier using reduced spectral characteristics of a cakes. As with the product above, the use of latent variables and principal components results in a general classification error of more than 10%. Using non-linear kernel principal components results in a zero classification error.



a) LV, e=25% b) PC, e=41% c) kPC, e=0%

Figure 7. Classification with the Naive Bayes Classifier for Cakes C3-C5

Table 1 shows the results of the Naïve Bayes classifier using the three methods to reduce the amount of data from spectral characteristics. The classification is made between samples with different percentages of additives. The general classification error presented as the value for all samples is determined. A value of up to 10% general classification error is selected as the criterion for successful separation between object areas. The results of data discrepancy between the classes show significantly lower classification errors using the nonlinear variant of the principal components, compared to the use of the other two methods to reduce the amount of spectral data. Expectedly, with a lower percentage of additives, the total classification error is higher than that between the control and those with a higher percentage of additives, where the overlap of the two classes is negligible.

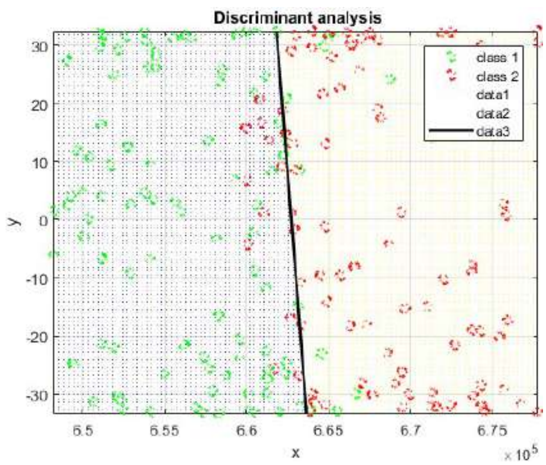
Table 1.

General classification error (e, %) using a Naïve Bayes classifier

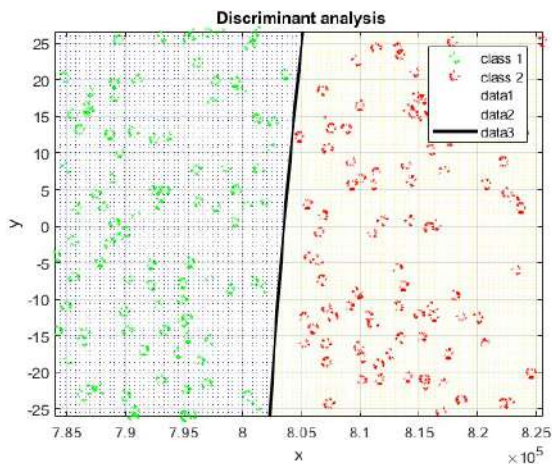
Cookies ASP				Cakes GPP			
Sample	LV	PC	kPC	Sample	LV	PC	kPC
P1-P2	38%	58%	0%	C1-C2	47%	62%	0%
P1-P3	28%	46%	0%	C1-C3	44%	49%	0%
P1-P4	22%	50%	0%	C1-C4	38%	50%	0%
P1-P5	14%	37%	0%	C1-C5	34%	44%	0%
P1-P6	3%	46%	0%	C2-C3	46%	50%	0%
P2-P3	37%	46%	0%	C2-C4	48%	61%	1%
P2-P4	33%	50%	2%	C2-C5	31%	44%	0%
P2-P5	21%	38%	0%	C3-C4	50%	50%	0%
P2-P6	7%	45%	0%	C3-C5	26%	41%	0%
P3-P4	47%	50%	0%	C4-C5	27%	49%	0%
P3-P5	28%	35%	0%	-	-	-	-
P3-P6	14%	43%	0%	-	-	-	-
P4-P5	33%	38%	0%	-	-	-	-
P4-P6	16%	45%	0%	-	-	-	-
P5-P6	14%	47%	5%	-	-	-	-

The analysis made with the Naïve Bayes Classifier revealed that an appropriate method for distinguishing baked product samples, depending on the percentage of additives, is the nonlinear variant of the principal components. This data was used to classify with a discriminant classifier and one using the support vector machines method.

Figure 8 shows examples of classification with a discriminant classifier. DA applied to non-linear PCA model data showed an inaccuracy of classification of both products with different additive amounts up to 11%.



a) P2-P4, Linear, e=11%



b) C2-C4, Linear, e=1%

Figure 8. Classification by kPCs with Discriminant Classifier

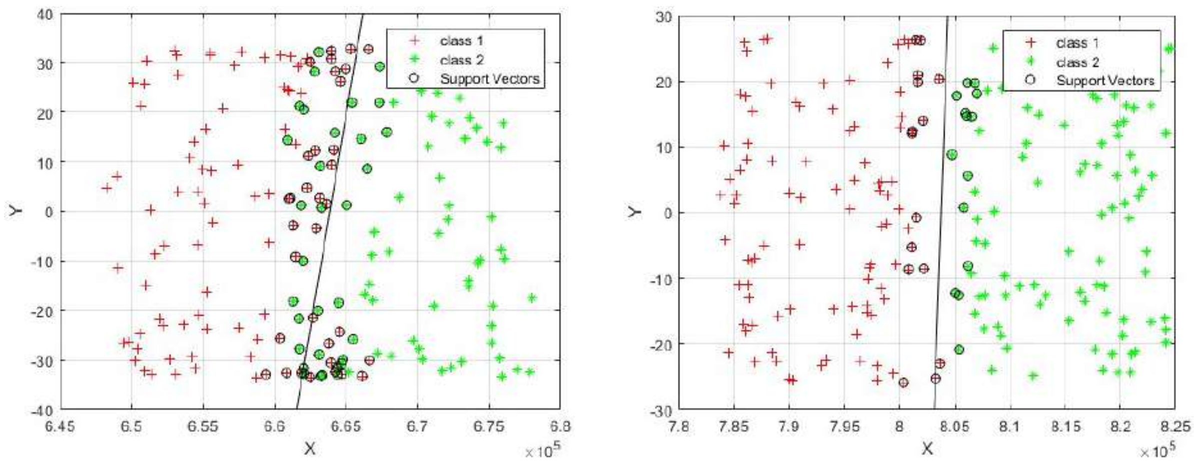
Table 2 shows results of the work of the Discriminant Classifier using a method to reduce the amount of data of the kPC spectral characteristics. For ASP-added cookies, low general classification error values are observed when differentiating all samples except between P2-P4 and P5-P6. In the classification of a GPP-supplemented cakes, a general classification error of 1% is observed between samples C2-C4. In addition to the small differences in the amount of additive in overlapping samples, other factors may also affect the separability, which with the amount of additive used may make specific changes to the product properties. Further studies need to be carried out to identify additional factors affecting the separability of baked product classes.

Table 2.

General classification error (e,%) using Discriminant Classifier

Cookies ASP						Cakes GPP					
Sample	L	DL	Q	DQ	M	Sample	L	DL	Q	DQ	M
P1-P2	0%	0%	0%	0%	0%	C1-C2	0%	0%	0%	0%	0%
P1-P3	1%	1%	1%	1%	1%	C1-C3	0%	0%	0%	0%	0%
P1-P4	0%	0%	0%	0%	0%	C1-C4	0%	0%	0%	0%	0%
P1-P5	0%	0%	0%	0%	0%	C1-C5	0%	0%	0%	0%	0%
P1-P6	0%	0%	0%	0%	0%	C2-C3	0%	0%	0%	0%	0%
P2-P3	0%	0%	0%	0%	0%	C2-C4	1%	1%	1%	1%	1%
P2-P4	11%	10%	11%	10%	11%	C2-C5	0%	0%	0%	0%	0%
P2-P5	0%	0%	0%	0%	0%	C3-C4	0%	0%	0%	0%	0%
P2-P6	0%	0%	0%	0%	0%	C3-C5	0%	0%	0%	0%	0%
P3-P4	0%	0%	0%	0%	0%	C4-C5	0%	0%	0%	0%	0%
P3-P5	0%	0%	0%	0%	0%	-	-	-	-	-	-
P3-P6	0%	0%	0%	0%	0%	-	-	-	-	-	-
P4-P5	0%	0%	0%	0%	0%	-	-	-	-	-	-
P4-P6	0%	0%	0%	0%	0%	-	-	-	-	-	-
P5-P6	27%	28%	26%	27%	27%	-	-	-	-	-	-

Figure 9 shows examples of SVM classifier classification. For this example, low values of the general classification error of up to 7% are observed using the kernel variant of the principal components. Using this classifier results in significantly smaller general errors than the discriminant analysis.



a) P2-P4, Linear, e=7% b) C2-C4, Linear, e=0%

Figure 9. Classification by kPCs with SVM Classifier

Table 3 shows the results of the operation of the SVM classifier using a method to reduce the data volume of the kPC spectral characteristics. For ASP-added cookies, low total classification error values are observed when distinguishing all samples. Again, as in the discriminant analysis, errors up to 17% were observed between P2-P4 and P5-P6. When classifying a GPP-added cupcake, a total classification error of 0%.

Table 3.

General classification error (e,%) using an SVM classifier

Cookies ASP					Cakes GPP				
Sample	L	Q	Poly	RBF	Sample	L	Q	Poly	RBF
P1-P2	0%	0%	0%	0%	C1-C2	0%	0%	0%	0%
P1-P3	0%	0%	0%	0%	C1-C3	0%	0%	0%	0%
P1-P4	0%	0%	0%	0%	C1-C4	0%	0%	0%	0%
P1-P5	0%	0%	0%	0%	C1-C5	0%	0%	0%	0%
P1-P6	0%	0%	0%	0%	C2-C3	0%	0%	0%	0%
P2-P3	0%	0%	0%	0%	C2-C4	0%	0%	0%	0%
P2-P4	7%	2%	2%	0%	C2-C5	0%	0%	0%	0%
P2-P5	0%	0%	0%	0%	C3-C4	0%	0%	0%	0%
P2-P6	0%	0%	0%	0%	C3-C5	0%	0%	0%	0%
P3-P4	0%	0%	0%	0%	C4-C5	0%	0%	0%	0%
P3-P5	0%	0%	0%	0%	-	-	-	-	-
P3-P6	0%	0%	0%	0%	-	-	-	-	-
P4-P5	0%	0%	0%	0%	-	-	-	-	-
P4-P6	0%	0%	0%	0%	-	-	-	-	-
P5-P6	17%	0%	3%	2%	-	-	-	-	-

An advantage of the methods used in the present work is that a nonlinear variant of the principal components of the spectral characteristics is used, whereby a recognition accuracy of 83-99% is obtained in the visible spectrum. Similar results were obtained by Jirsa et al. [11], who state that spectral characteristics can be used to predict changes in the composition of bread products with an accuracy of up to 99%. Using multispectral images Andresen et al. [2] indicate that at two wavelengths of spectral characteristics 395 and 525nm, a strong relationship with the amount of melanoids in biscuits is observed in the visible spectrum.

From the obtained results and analyzes it can be pointed out that it is necessary to make further studies related to the effect of changes in the composition of biscuits and cupcakes with food-by-product additives and their relation to their spectral characteristics.

4. Conclusion

Small differences are observed with the addition of secondary products from the food industry (ASP and GPP), on spectral characteristics of the surface of the baked products.

In addition to the different possibilities for evaluating the spectra of the baked products, it has been found that the direct application of spectral characteristics to differentiate baked products, depending on their composition, is inappropriate because of the strong overlap of experimental data.

The results of the separation of object areas of bakery products are highly dependent on the method of feature extraction and reducing the input data, as well as on the method of classification.

The best results are obtained using kernel variants of PCA. For different classifiers, the general classification errors range from 0% to 17%. When using the kPCA, the two areas of points corresponding to the spectral characteristics of the two areas with different amounts of additives are sufficiently compact and spaced apart, which also explains the results obtained for separating these areas by the classifiers used.

The methods used for classification with the best precision work SVM with polynomial and radial-basis function. With those two non-linear functions of SVM, it is practically possible to distinguish data in both ASP-added cookies and GPP-added cakes with a general classification error not exceeding 10%.

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ВЛИЯНИЕ НА ДОБАВКИ ОТ ОТПАДЪЧНИ ХРАНИТЕЛНИ ПРОДУКТИ ВЪРХУ СПЕКТРАЛНИ ХАРАКТЕРИСТИКИ НА ХЛЕБНИ ИЗДЕЛИЯ

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Резюме: Работата в тази статия има за цел да се определи влиянието на добавените отпадъчни хранителни продукти върху спектралните характеристики на хлебни изделия. Анализирани са бисквити с добавена ябълкова пудра и кекс с прах от гроздови семки. Използват се три метода за редуциране на обема от данните на спектралните характеристики: латентни променливи, линеен и нелинеен вариант на главните компоненти. Изборът на метод за редуциране на обема от данни се базира на класификация с Наивен Бейсов класификатор. Данните от избрания нелинеен вариант на главните компоненти се използват за класифициране с дискриминантен анализ и метод на опорните вектори. Резултатите от оценката на разделимостта на обектите области на хлебните изделия, силно зависят от метода на извличане на характерни свойства и намаляване обема на входните данни, както и от метода за класификация. По-добри резултати се получават с нелинеен вариант на метода на опорните вектори, в сравнение с неговия линеен вариант и дискриминантния анализ.

***Ключови думи*:** Бисквити, кекс, отпадъчни хранителни продукти, спектрални характеристики, редуциране обема от данни, класификация

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