

НОВЫЕ МАТЕРИАЛЫ И НАНОТЕХНОЛОГИИ MATERIAL SCIENCE AND NANOTECHNOLOGIES

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Improving the algorithm for processing data from multisensor system in tasks of determining quality parameters in vegetable oils

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Abstract

The effective functioning of modern production systems is impossible without using of methods for processing and analyzing data continuously generated during operation. Limitations imposed on the speed and precision of determining the required indicators lead to the need of optimizing the algorithms used. Multisensor systems, as a rule, have an excessive number of cross-sensitive sensors, and their signals can be used to determine various indicators of a similar physical nature. The purpose of the study is to improve the algorithm for processing multidimensional data from multisensor systems. Principal component analysis was applied as part of the developed algorithm for the formation of informative features. Partial least squares regression was used to build regression models. The data set for approbation of proposed approach was obtained through potentiometric measurements using a digital mV-meter. An experiment is described using a multisensor system called “electronic tongue”, consisting of 12 cross-sensitive potentiometric sensors. In the experiment, real samples of vegetable oils acted as analyzed objects. Regression models were built to determine three quality indicators of vegetable oils: peroxide value, para-anisidine value and total tocopherol concentrations. The results of the study were compared with known scientific works. A comparative analysis allowed us to conclude that using of the most informative sources selected according to the proposed algorithm can significantly reduce the root mean square error of prediction. The results obtained can be used both in systems for identifying deviations in production processes in “Industry 4.0” enterprises, and for expressly identifying counterfeit products.

Keywords

quantitative analysis, quality control, vegetable oils, potentiometric sensors, multisensor system, time series, principal component analysis

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Совершенствование алгоритма обработки данных от мультисенсорной системы в задачах определения показателей качества растительных масел

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Аннотация

Введение. Эффективное функционирование современных производственных систем невозможно без применения методов обработки и анализа, непрерывно формируемых в процессе эксплуатации данных. Ограничения, накладываемые на скорость и точность определения искомых показателей, приводят к необходимости оптимизации применяемых алгоритмов. Мультисенсорные системы, как правило, обладают избыточным количеством перекрестно-чувствительных сенсоров, при этом их сигналы могут применяться для определения

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различных схожих по физической природе показателей. Целью исследования является совершенствование алгоритма обработки многомерных данных от мультисенсорных систем. **Метод.** В составе разработанного алгоритма формирования информативных признаков применен метод главных компонент. Для построения регрессионных моделей использован метод регрессии частичных наименьших квадратов. Массив данных для проверки предложенного подхода получен в ходе потенциометрических измерений с использованием цифрового милливольтметра. Проведен эксперимент с использованием мультисенсорной системы типа «электронный язык», состоящей из 12 перекрестно-чувствительных потенциометрических сенсоров. В эксперименте в качестве анализируемых объектов выступали реальные образцы растительных масел. **Основные результаты.** Построены регрессионные модели для определения трех показателей качества растительных масел: перекисного числа, пара-анизидинового числа и общего содержания токоферолов. Результаты исследования сопоставлены с известными научными работами. **Обсуждение.** Сравнительный анализ позволил сделать вывод о том, что использование отобранных по предложенному алгоритму наиболее информативных источников позволяет значительно снизить среднеквадратичную ошибку прогнозирования. Полученные результаты могут применяться как в системах выявления отклонений производственных процессов на предприятиях «Индустрии 4.0», так и для экспресс-выявления фальсификатов продукции.

Ключевые слова

количественный анализ, контроль качества, растительные масла, потенциометрические сенсоры, мультисенсорная система, временные ряды, метод главных компонент

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Introduction

“Industry 4.0” involves a new approach based on the mass introduction of information technology into industry [1]. Cyber-physical systems (CPS), in turn, are the basis for the implementation of many modern innovative solutions [2].

Monitoring and control components [3] connect the CPS with the physical world through sensors and transducers for monitoring physical components and actuators for controlling them [4]. Fig. 1 shows the general model of the CPS which includes monitoring and control units.

The data array from the monitoring system characterizes a specific production process or analyzed object. In both cases, from the entire set of sensors, it is important to select a fixed set for the required monitoring or analysis purposes, which determines the relevance of the problem being solved. The improvement of multisensor systems, in particular systems such as “electronic tongue” and “electronic nose”, makes it possible to effectively use them as an array of sensors for CPS.

The modern development of sensor technologies, the emergence of new and improvement of existing methods

and measuring instruments leads to increased precision and sensitivity of object analysis. At the same time, the growing amount of signal information coming from monitoring systems requires modernization of methods for processing multidimensional data in order to optimize computational costs and increase the speed of their processing. In this regard, the development of models and methods that make it possible to select the most informative ones for the goals and objectives of analysis from the available number of sensors is of particular relevance.

Problem statement

The initial feature space H represents the entire set of sensors (mechanical, electrical, acoustic, optical, physicochemical, and others) available for a given CPS configuration that record certain system parameters. Obviously, it is extremely important to identify features that allow achieving maximum precision and recall of the analysis at acceptable computational costs. In the case of large industrial productions implementing “Industry 4.0” technologies, the number of such sensors can reach hundreds and even thousands for each link of the system.

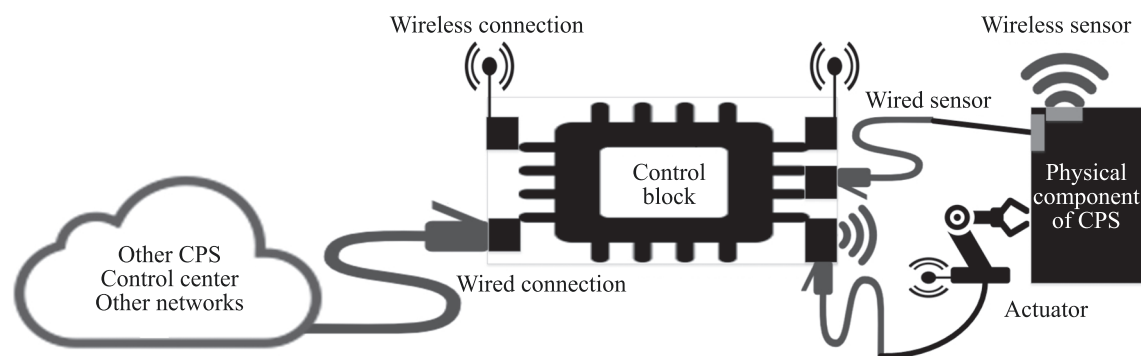


Fig. 1. General model of CPS

It is required to transform the original feature space $H = (f_1, f_2, \dots, f_n)$ into the space:

$$H^* = (f_1, f_2, \dots, f_s), \text{ wherein } I_{f1} \geq I_{f2} \geq \dots \geq I_{fs},$$

where n is the number of gradations of the attribute (dimension of the original data space); s — number of selected most informative features; $f_1, f_2, \dots, f_s$ — selected most informative features; I_{fi} — informativeness of the i -th feature.

Proposed approach

This research continues the implementation of the approach proposed in [5] and shows the possibility of its application in other types of CPSs.

Principal Component Analysis (PCA) is widely used to reduce the dimensionality of source data [6]. In most studies, PCA is used as preprocessing [7], in these cases the original multidimensional feature space is transformed into the space of principal components (PC). In this study, in contrast to well-known works, PCA is proposed to be used to calculate the informativeness of each feature (source of information about the analyzed objects).

Data matrix $\mathbf{X}$ represents the results of measuring some object parameters over time:

$$\mathbf{X} = \begin{pmatrix} x_{1,1} & x_{1,2} & \dots & x_{1,n} \\ x_{2,1} & x_{2,2} & \dots & x_{2,n} \\ \dots & \dots & \dots & \dots \\ x_{m,1} & x_{m,2} & \dots & x_{m,n} \end{pmatrix},$$

where m is the number of data vectors (number of rows); n — initial dimension of the data space (number of columns).

Before using PCA to analyze the training sample, it is necessary to perform autoscaling (centering and normalizing) of the data [8]. Each line of the matrix X in this case — are the values of preprocessed data, composed of parameters obtained from the system sensors at a discrete point in time.

The decomposition of the matrix $\mathbf{X}$ in the form of a matrix equation using the principal component analysis method can be represented as follows:

$$\mathbf{X} = \mathbf{TP}^T + \mathbf{E},$$

where index “ T ” is a transposition operation, as a result of which the matrix is rotated relative to its main diagonal, $\mathbf{T}$ is the matrix of scores:

$$\mathbf{T} = \begin{pmatrix} t_{1,1} & t_{1,2} & \dots & t_{1,k} \\ t_{2,1} & t_{2,2} & \dots & t_{2,k} \\ \dots & \dots & \dots & \dots \\ t_{m,1} & t_{m,2} & \dots & t_{m,k} \end{pmatrix}.$$

Each row of the matrix $\mathbf{T}$ is a projection of the preprocessed data vector onto k principal components, number of rows — m (number of time series), number of columns — k (number of PC vectors selected for projection) [9]. $\mathbf{P}$ — loadings matrix:

$$\mathbf{P} = \begin{pmatrix} p_{1,1} & p_{1,2} & \dots & p_{1,k} \\ p_{2,1} & p_{2,2} & \dots & p_{2,k} \\ \dots & \dots & \dots & \dots \\ p_{n,1} & p_{n,2} & \dots & p_{n,k} \end{pmatrix}.$$

Each column of the matrix $\mathbf{P}$ is a vector of principal components, the number of rows is n (the dimension of the original data space), the number of columns is k (the number of PC vectors selected for projection) [9]. The loadings values p belong to the range $[-1; +1]$ and reflect the influence of a specific source variable on a given PC. $\mathbf{E}$ — errors of residuals matrix: $\mathbf{E} = \mathbf{X} - \mathbf{TP}^T$.

Before calculating the informativeness of features, it is necessary to solve the problem of choosing the number of PC (k). To do this, sequentially, starting from unity, the values of explained residual variance (ERV) are calculated for each value of k using the formula:

$$ERV = 1 - \sum_{i=1}^m \sum_{j=1}^n e_{ij}^2 / \sum_{i=1}^m \sum_{j=1}^n x_{ij}^2,$$

where e_{ij} are elements of the matrix $\mathbf{E}$; x_{ij} — elements of matrix $\mathbf{X}$.

Decision rule for choosing k : $ERV_k \geq \varepsilon$, where ε is chosen empirically depending on the specific CPS. Then the informativeness of the i -th feature with k principal components is calculated using the matrix $\mathbf{P}$ according to the formula:

$$I_{fi} = \sqrt{\sum_{j=1}^k p_{ij}^2}. \quad (1)$$

Source identifiers are ordered by informativeness $I_{f1} \geq I_{f2} \geq \dots \geq I_{fn}$, and according to Guttman-Kaiser criterion [10], s sources are selected whose informativeness is bigger than the average informativeness:

$$I_{fi} > \frac{1}{n} \sum_{i=1}^n I_{fi},$$

where I_{fi} is the informativeness of the i -th source; $\frac{1}{n} \sum_{i=1}^n I_{fi}$ — average informativeness of all sources under consideration; $i = 1, \dots, n$.

The scheme of the algorithm for the formation of informative features in problems of quantitative analysis of objects is presented in Fig. 2.

Experiment

In the experiment, real samples of vegetable oils were used as analyzed objects. Using the methods described in [11], an array of twelve cross-sensitive potentiometric sensors was manufactured. The composition of the sensors is given in Table 1.

Fig. 3 shows the appearance of the sensor array.

Potentiometric measurements were carried out in the following galvanic cell:



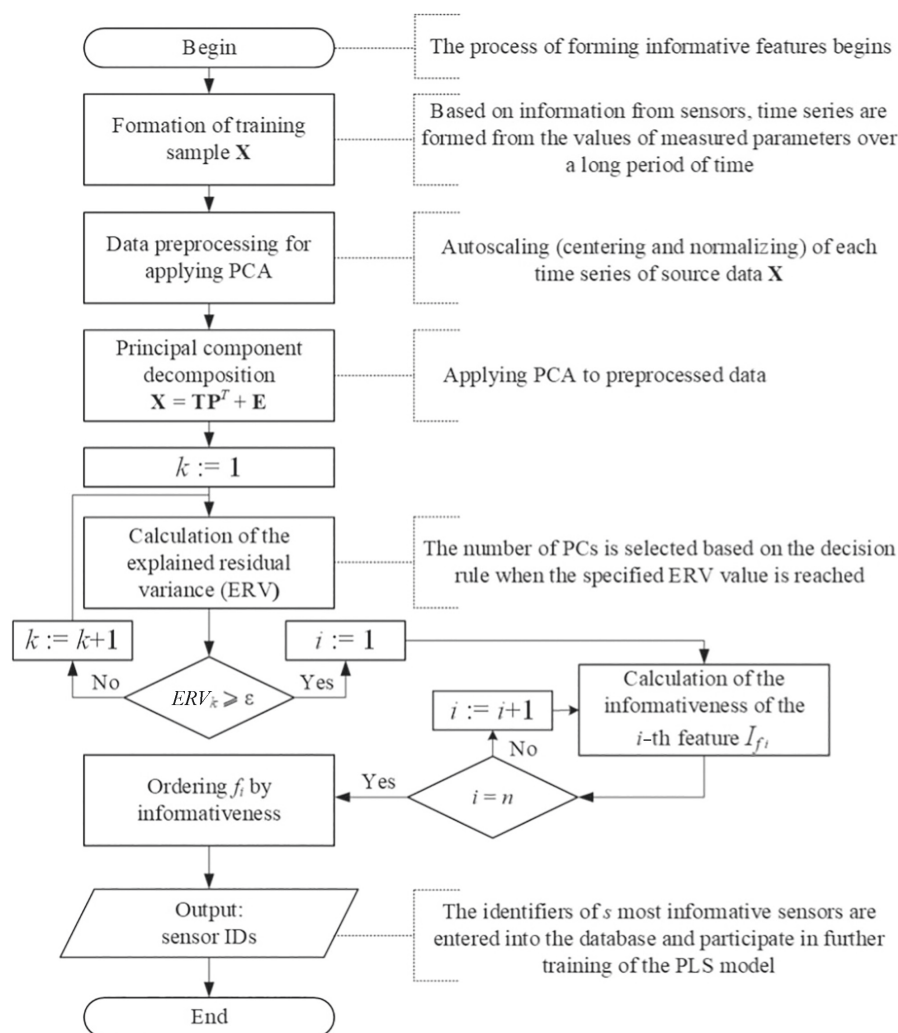


Fig. 2. Algorithm for the formation of informative features

The reference electrode was an ESr-10101 (Izmeritel'naya tekhnika, LCC, Moscow, Russia) silver chloride electrode filled with a saturated solution of

potassium chloride. Electrode responses were recorded after 3 min of equilibration in each analyzed emulsion on high input impedance multi-channel digital mV-meter KHAN-11 (Sensor Systems, LLC, St. Petersburg, Russia) connected to the personal computer for data acquisition and processing. Between measurements, the electrodes were stored in air.

Table 1. Composition of the array of sensors used in the experiment

Sensor identifier	Membrane material
A7	Polycrystalline mixture AgCl-Ag ₂ S
A14	LaF ₃ ceramic membrane doped with Eu
A25	Polycrystalline mixture AgI-Ag ₂ S
A26	Polycrystalline mixture AgBr-Ag ₂ S
A27	Polycrystalline mixture Ag ₂ S
G1	Metal electrode Au
G2	Metal electrode Sb
G4	Chalcogenide glass membrane Cu-Ag-As-Se
G5	Chalcogenide glass membrane Cu-Ag-As-Se-Te
G10	Chalcogenide glass membrane CdI ₂ -AgI-As ₂ S ₃
G11	Chalcogenide glass membrane PbS-AgI-As ₂ S ₃
G13	Chalcogenide glass membrane Ag ₂ S-As ₂ S ₃



Fig. 3. Appearance of sensors

The composition of the analyzed objects and the measurement technique are described in detail in [12]. The analyzed parameters were peroxide values, para-anisidine values and total tocopherols concentrations. Knowledge of these parameters can serve as an important indicator of the quality of vegetable oils and their possible falsification [13, 14]. For all samples, reference data were obtained for each of the above parameters based on standard methods. Multivariate data processing was performed using MATLAB R2023b (The MathWorks, Inc., USA) software.

Results and discussion

The model for the formation of informative features was applied to time series consisting of sensor responses immersed in vegetable oil samples of different compositions. The specified ERV value corresponded to the number of PCs $k = 5$. For clarity, Fig. 4 shows a graph of loadings for PC1 and PC2, which have a large impact on the final value of informativeness. As the absolute values of the coordinates of a point increase, the informativeness of the corresponding sensor increases.

The informativeness of the features according to the developed algorithm is calculated using formula (1) and is presented in Fig. 5. The average informativeness ($\bar{I}$) was 0.611. The most informative features are highlighted in blue on the histogram. Red-ox sensitive sensors carry the most information about the composition of the analyzed samples, which is consistent with the operating principles of the above sensors.

Of the twelve sensors in the array, the informativeness of five turned out to be higher than the average informativeness, which made it possible to significantly reduce the number of features used to build a classification and regression model. Reducing the computational costs of processing a data array has made it possible to increase the speed of response to production incidents.

Interpretation of multisensor system response was performed using partial least squares regression (PLS) [15]. The root mean square error (RMSECV) [16] was calculated according to the following formula, full cross-validation was used to calculate the indicator:

$$RMSECV = \sqrt{\frac{\sum_{o=1}^w (y_{o,pred} - y_{o,real})^2}{w}},$$

where $y_{o,pred}$ — predicted value for the o -th oil sample; $y_{o,real}$ — values for the o -th oil sample obtained based on the reference methods; w — total number of samples.

Table 2. Results of applying PLS models with and without the developed method

Parameter (it range)	Method	Slope	Offset	RMSECV	R ²
Peroxide value (0–4), mEq/kg	Developed method	0.99	0.01	0.1	0.99
	Result from [12]	0.97	0.05	0.5	0.89
Para-anisidine value (0.5–3.8)	Developed method	0.97	0.17	0.2	0.91
	Result from [12]	0.76	0.43	0.8	0.67
Total tocopherols content (37–100.7), mg/100 g	Developed method	0.96	3.71	4.7	0.95
	Result from [12]	0.80	11.50	10.0	0.83

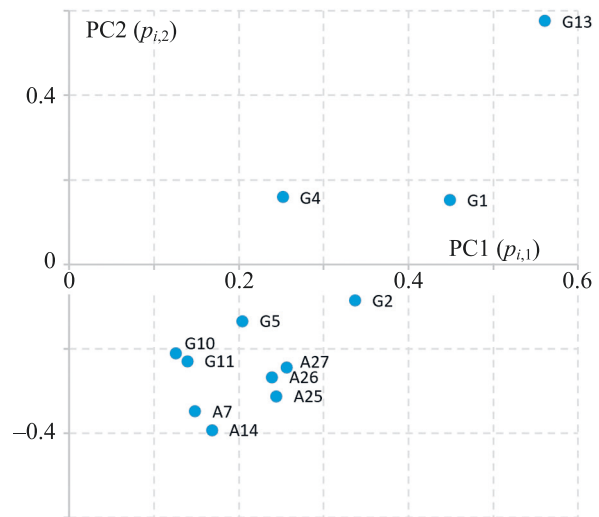


Fig. 4. Principal component analysis loadings plot for sensors used in the experiment

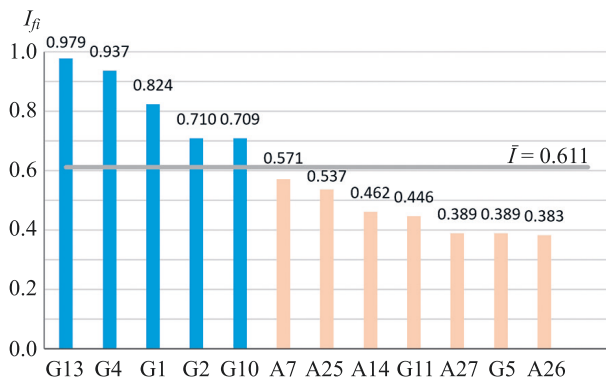


Fig. 5. Informativeness values for each sensor. $\bar{I}$ — average informativeness

Table 2 provides a comparative analysis of PLS models obtained using the developed algorithm for generating a list of the most informative features and without it.

Thus, when using the developed method, due to the removal of noise sources of information, the root mean square error is noticeably reduced. The values of the R² metric tell us that the predictor variables in the model (sensor signals) after applying the method are able to explain 91–99 % of the fluctuations in the measured technological indicators.

Conclusion

This research proposes a method and describes an algorithm for the formation of informative features in problems of quantitative analysis of objects using vegetable oils as an example. The developed method makes it possible to increase the precision, recall and speed of multiclass classification and regression at subsequent stages. The proposed method is invariant to the dimensions and orders of magnitude from which the time series fed to the input of the algorithm are composed.

The method was tested on a data set obtained during an experiment with real samples of vegetable oils. The paper describes the composition of the sensors of the multisensor system used and the potentiometric measurement technique.

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The obtained results were compared with previously known ones. Comparison allows us to conclude that removing noise information from individual sources can significantly reduce the root mean square error, which will allow the developed method to be used both in systems for detecting deviations in production processes and for the purpose of expressly identifying counterfeits.

During the research, an interdisciplinary approach was used to expand the capabilities of modern methods of quantitative analysis of objects at “Industry 4.0” facilities, where there is a colossal number of sensors and it is necessary to determine a set of signals that make it possible to obtain useful information about the analyzed object or processes.

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