Integrated Machine Learning Models for Bakery Product Defect Prediction

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Keywords: Defect Prediction, Machine Learning Models, Correction, Bakery Products.

Abstract: The paper discusses the development of a model for predicting the probability of occurrence of defects in bakery products using a set of input variables at different stages of the technological process. The model is based on the analysis of data including control variables, such as oven temperature and humidity, as well as disturbance variables characterizing the properties of flour, the dough preparation process and baking of products. Based on the results of the study, a GMM-based model was selected, which demonstrated the highest accuracy, with the achieved Precision and Recall values equal to 1.0 for the class of defective products, which indicates high correctness of forecasts. In terms of Log-Likelihood, the model demonstrated a large difference between the classes, which confirms its ability to accurately classify both defective and non-defective products. The proposed model is an effective tool for predicting defects and optimizing process parameters. It allows you to adjust control variables, such as temperature and humidity, to reduce the amount of defects, ensuring stability of product quality. The article also proposes different methods for adjusting the values of control variables based on historical data. This allows for optimization of the technological process and improvement of the quality of bakery products in real-time production conditions.

1 INTRODUCTION

The development of artificial intelligence, digitalization of all stages of production, implementation of digital twins, organization of processes according to the concept of intelligent production, requires the development and use of models of varying complexity and type. There is also a tendency to increase the complexity of emerging engineering and technical problems. Increasingly, for their accurate and successful solution, it is necessary to combine several different models. Therefore, integrated models are often used, providing solutions to complex problems based on a systems approach by combining several individual models into a single structure, taking into account the relationships between different components of the system [1].

The modern food industry is faced with a constant increase in product quality requirements, especially in the bakery industry. One of the key tasks is to minimize the defects of bakery products that occurs due to imperfections in the technological process, in particular at the baking stage. This stage is critically important, since the structure, taste, texture and appearance of the finished product depend on it. Realtime defect prediction and adaptive control of baking parameters are promising approaches to improving product quality and reducing defects. For this purpose, it is advisable to use defect models that allow you to analyze, predict, prevent the occurrence in time and reduce the total number of defects and/or discrepancies in production processes [2].

The combination of defect models in integrated models allows for local analysis of defects taking into account the interrelations existing in the existing production system. In particular, to identify the impact of changes in the quality indicators of raw materials, the operation of process equipment or working conditions on the total number of defects [3] or to analyze the systemic causes of defects through a multifactorial approach that takes into account technologies and external influences [4, 5]. The combination of these two approaches ensures effective quality control of final products and semifinished products, reduces losses, downtime, unplanned repairs and increases productivity.

The object of the study is the technological processes of manufacturing bakery products at the enterprise, including key variables of dough preparation, dough piece aging and baking, which affect the defects of the final product.

The subject of the study is methods for optimizing the technological process of preparing bakery products using machine learning models that allow predicting and monitoring product defects, automating the selection of technological parameters and adapting the process to changing production conditions.

The purpose of the study is to develop and substantiate approaches to optimizing the bakery production process using machine learning models, which ensures the minimization of defective products at the baking stage and increases the efficiency of production processes in general.

This paper discusses the development of a control system that uses machine learning to predict bakery product defects based on process characteristics and to correct control actions in order to minimize defects.

2 LITERATURE REVIEW

There are various models, methods and tools that help productions to identify and manage defects during their technological processes [6]. Combining several separate adequate models or approaches into a single structure provides a significant improvement in solving complex problems where it is necessary to take into account many different factors and relationships. This is confirmed by the results of research by scientists in various subject areas. This is due to the main characteristics of integrated models: multi-modeling, interdisciplinarity, adaptability, system approach, the ability to conduct various types of testing and simulations in complex systems.

Thus, Integrated Assessment Models (IAMs) determine hydrogen demand through the analysis of technology competition for energy services [7], but their low spatial and temporal resolution limits their application in global hydrogen trade. The presented framework combines IAMs with high-resolution models, optimizing the production, storage and transmission of hydrogen and electricity, allowing the exploration of future trade scenarios.

Integrated models incorporating multiple pharmacodynamic variables are used to support drug development, in particular, dosing optimization and study strategy in different patient subgroups. The authors [8] provide current examples of such models, key aspects and benefits of their application, and prospects for the development of individualized development of anticancer drugs. The use of integrated models in industry is actively developing. The study [9] focuses on an integrated planning model for electrical wiring manufacturers, which improves the synchronization of production processes and product inventories, ensuring uninterrupted supply for the automotive sector. The use of a model based on integer programming showed a significant reduction in lead time, which proves its effectiveness and the importance of collaborative planning in supply chains.

Integrated models are also used to analyze and determine optimal digital transformation strategies (Industry 4.0) in the automotive industry, taking into account technological, environmental and business aspects. They provide a comprehensive approach to assessing companies' readiness, developing new business models and taking into account sustainability in the process of implementing digital technologies [10]. Integrated models can be used to create a sustainable agri-food supply chain, combining cultivation, processing and distribution solutions to minimize costs and environmental impact. Using multivariate analysis, geospatial data and mathematical modeling, the study identifies optimal location, production and logistics strategies, ensuring profit and employment maximization while adapting to uncertain conditions [11].

Therefore, to improve the efficiency of defect tracking and processing, it is advisable to use integrated models that take into account data on various defects, their life cycle, historical data, the influence of external factors, available resources for working with defects, etc. Such modeling is used to determine the causes and evaluate defects, isolate failures and analyse their impact.

Defect modeling is used to identify failure causes and estimate defects by isolating faults and analyzing their impact. This approach significantly improves the accuracy of estimates, reduces the number of possible defects and the area of interest, allowing for effective problem detection even under limited data conditions [12].

Recent research in defect detection highlights the limitations of traditional image processing under complex textures and varying lighting conditions. As a result, deep learning methods are increasingly applied due to their ability to automatically extract features and handle complex data [13], [14]. These methods are effective in various quality control scenarios, including surface and X-ray image analysis [14]. However, challenges such as data imbalance, limited sample size, and the need for realtime processing remain relevant [13], [15]. Overall, the integration of non-contact technologies with MLbased methods represents a promising direction for developing intelligent inspection systems [15].

One of the powerful areas of work with defects is the use of anomaly detection methods [16]. Anomaly detection is a method and technique for detecting and identifying atypical or deviant events or observation data that do not correspond to the expected process. Such methods are widely used in data analysis, cybersecurity, predicting system failures, quality control, etc.

The main methods for detecting anomalies can be distinguished: statistical methods based on the analysis of data samples and the identification of deviations outliers and from the normal distribution [17]; methods based on time series for data that change over time [18]; methods based on distances [19] and density [20] for working with data in multidimensional space; Bayesian methods that estimate the probability of a point being abnormal based on cause-and-effect relationships in the data [21]; when working with network nodes, it is convenient to use graph-based methods [22]; when analyzing complex data structures, machine learning methods have proven to be the best for determining various deviations [23-25].

Therefore, the advantages of using integrated models include their ability to take into account the maximum number of interdependencies between the components of the system and the processes occurring in it; they also make more accurate forecasts and provide a better basis for decisionmaking. This also causes certain difficulties in working with these models: the need to use highquality data for their development; high computational requirements; difficulties may arise when integrating heterogeneous models.

3 PREPARATION AND PRELIMINARY DATA ANALYSIS

In modern bakery production, a significant proportion of product defects are detected at the final stage during baking. This is due to the fact that visual defects, such as uneven rise, excessive density or undesirable crust color, become noticeable only at the stage of thermal treatment. In such cases, the production process is forced to end without the possibility of correction, which leads to a loss of resources such as raw materials, energy and time. In addition, timely identification of defective products requires qualified specialists or automated visual inspection systems.

The article proposes an integrated approach to predicting defects at early stages of production, based on the characteristics of flour, dough and proofing process parameters. Using machine learning models will allow these characteristics to be analyzed to determine the probabilities of a defect even before the baking stage, allowing for early process termination or adjustments. This will not only improve production efficiency, but also minimize the costs associated with recycling or disposal of defective products.

3.1 Data Collection and Pre-Processing

To build a forecasting model, data were collected, including all measured technological product change portions at the stages of dough preparation, dough piece standing and baking. These data were obtained from automated production line control systems. At the stage of preliminary data processing, noise is removed, and values are normalized for subsequent use in machine learning models. For this, standard data processing methods are used, in particular, standardization and filling in missing values.

In addition to automated approaches to identifying emissions, each of the calculated emissions was additionally examined manually, taking into account the features of the technological process and the specifics of production. This made it possible to take into account the possible causes of emissions and correctly make decisions on their removal, correction or preservation in the sample for further analysis.

When selecting features for building the model, an individual approach was applied to each variable, regardless of the level of correlation with other features. Both statistical characteristics and the technological significance of each feature for predicting defects were taken into account. This made it possible to form a set of variables reflecting real physical and chemical processes at all stages of production.

The total dataset contains 321 samples, of which 48 are defective (class label y = 1) and 273 are nondefective (class label y = 0). This indicates a class imbalance, which was taken into account during model selection and evaluation.

Table 1 shows the selected variables, and Figure 1 shows their correlation matrix. Note that x_1, \ldots, x_4 determine the initial quality of the raw

material, which has a significant impact on the formation of the dough structure. For example, flour strength (x_3) correlates with the sugar-forming capacity of the dough during fermentation, and gasforming capacity (x_2) is closely related to the rise of the dough. The group of variables $x_5, ..., x_7$ describes the main technological variables of dough mixing and fermentation. In particular, water consumption (x_5) affects the consistency of the dough, while titran acidity (x_7) reflects the activity of enzymatic processes and determines the taste. At the stage of proofing of dough pieces, two variables were selected: humidity and weight of the dough piece (x_8, x_9) , which have a direct impact on the plasticity and readiness of the dough for baking. The high correlation of these variables with the quality of the finished product allows them to be used as predictors. Baking variables such as temperature and humidity in the humidification zone (x_{10}, x_{11}) , have a significant impact on crust formation, baking and bread color. Deviations in these variables often result in defects.

Table 1:	Input and	output v	variables	of the mo	del.

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Raw material or process	Variable notation	Variable decryption	
	$x_1(z_1)$	Quantity and quality of gluten	
Properties of flour	$x_{2}(z_{2})$	Gas-forming capacity	
	$x_{3}(z_{3})$	Flour strength	
	$x_4(z_4)$	Sugar-forming capacity	
Preparing the dough	$x_{5}(z_{5})$	Water consumption	
	$x_{6}(z_{6})$	Dough fermentation time	
	$x_{7}(z_{7})$	Titric acidity of the dough	
Proofing the dough	$x_8(z_8)$	Dough piece moisture content	
	$x_{9}(z_{9})$	Dough piece weight	
Baking	$x_{10}(u_1)$	Humidity in the oven and in the humidification zone	
	$x_{11}(u_2)$	Baking temperature	
	у	Defect $[0, 1]$ (0 – no defect, 1 – defect)	

The mathematical model is represented by the following (1):

$$y = h(\overline{x}), \, \overline{x} = [x_1, x_2, \dots, x_{11}],$$
 (1)

where h() – model (hypothesis); y, x_i – the inputs and output of the model, respectively (Table 1).

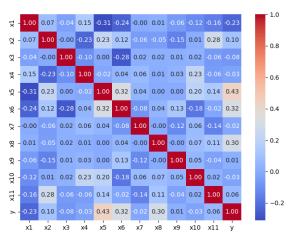


Figure 1: Visualization of process variable correlations.

3.2 Selection of Model Construction Methods

Due to the small amount of data with defective products (y = 1), the model is based on data only for non-defective products (y = 0), focusing on identifying patterns in this data. Consider the parallel coordinates plot (Fig. 2) showing the change in input variables for defective and non-defective products. It is clear that the values of some variables have stable levels, while others vary significantly, but no patterns are observed. Figure 3 shows that the non-defective product data is distributed compactly and without clearly visible clusters. This indicates that: dimensionality reduction methods (PCA) can be used to eliminate correlated variables.

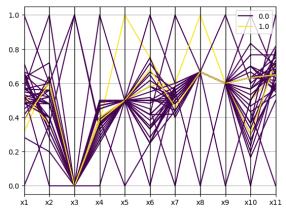


Figure 2: Parallel coordinates graph.

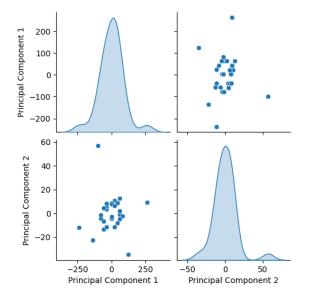


Figure 3: Principal component distribution densities for y = 0.

Thus, several methods can be proposed for constructing a model that do not require clear clusters or explicit boundaries for separation:

- Gaussian Mixture Model (GMM) –is one of the best methods for detecting anomalies when data can be represented as a mixture of several normal distributions.
- Isolation Forest It is an effective algorithm for anomaly detection that works particularly well in high-dimensional spaces and for identifying anomalies even when data clusters are not obvious.
- 3) One-Class SVM (Support Vector Machine) The method constructs a hyperplane separating "normal" data from anomalous data.
- 4) Local Outlier Factor (LOF) the method calculates the relative density of a point relative to its neighbors. If a point has a much lower density than its neighbors, it will be considered an anomaly. This works well when the anomalies are local.
- 5) k-Nearest Neighbors (k-NN) can be used to detect anomalies by comparing the distances between points. If a point is too far from its nearest neighbors, it can be considered an anomaly.
- 6) Autoencoders is a type of neural network that learns to reconstruct input data. It is suitable for working with multidimensional data, when there are complex relationships between features.

The Gaussian Mixture Model (GMM) is an optimal choice for this task because it can effectively

model complex data distributions where there are no clear clusters or boundaries between normal and abnormal points. By being able to describe data as a mixture of several normal distributions, GMM can detect abnormal points that deviate from the underlying distribution. This is especially useful in situations where the number of defective points is limited and where traditional methods based on clear separations or clustering may be less effective. GMM can work with small amounts of data and accurately detect anomalies, making it the most suitable method for this task. In addition, the choice of GMM for this task is determined by the specifics of the process and the nature of the data. In particular, GMM is able to effectively work with multidimensional data that have a complex structure with possible latent groups. At the preliminary analysis stage, the distribution of input features showed the presence of mixed distributions, which further confirmed the feasibility of using GMM. For comparison, other methods were also tested - One-Class SVM, Isolation Forest and ensemble methods (for example, Random Forest for classification). GMM demonstrated high accuracy and stability with a small amount of defective data, which is important for production conditions, where defects are rare events.

To make a rational choice, metrics such as the difference in logarithmic likelihoods between individual Log-Likelihood classes and precision/recall on test data will be used to evaluate the quality of forecasting and hyperparameters of the GMM model.

After building and testing the model in laboratory conditions, the system will be tested in real bakery enterprises. Testing includes collecting additional data and adjusting the models to ensure their effective application in real production conditions.

4 MODELING OF ANOMALIES DETECTION AND COMPARISON OF RESULTS

The modeling process was performed using the Python programming language, using the pandas, matplotlib, seaborn and sklearn libraries. Colaboratory (Google) was chosen as the programming environment.

The process of tuning the GMM hyperparameters (the number of components n_components and the type of covariance matrix) was performed based on cross-validation with optimization according to the criterion of minimizing the logarithmic likelihood (Log-Likelihood) for non-rejected data. Analysis of the test models showed that for 4 components with a full covariance matrix (covariance_type='full') the best balance between sensitivity and specificity of the model is achieved. This choice is consistent with the physical nature of the process, where each component can correspond to a separate technological state or a group of production conditions.

Based on the preliminary analysis, as well as through modeling, the following models were selected:

- Model 1: GMM by 2 principal components (PCA) with the number of Gaussian components n_components=5 and with the type of covariance matrix covariance_type= 'full';
- Model 2: GMM by 2 principal components (PCA) with the number of Gaussian components n_components=7 and with the type of covariance matrix covariance_type= 'full';
- Model 3: GMM for all features with the number of Gaussian components n_components=3 and with the type of covariance matrix covariance_type= 'full';
- Model 4: GMM for all features with the number of Gaussian components n_components=4 and with the type of covariance matrix covariance_type= 'tied';
- Model 5: GMM for all features with the number of Gaussian components n_components=4 and with the type of covariance matrix covariance_type= 'full'.

For each model, an optimal wear threshold was selected based on the logarithmic probability estimate of training and test points. This allows to determine the most optimal threshold for detecting anomalies in unknown data.

Table 2 shows the simulation results for different model configurations in terms of Precision and Recall metrics, as well as the minimum Log-Likelihood values. Model 1 shows a medium balance between prediction accuracy and anomaly detection ability. Precision is 0.8, indicating that most of the predicted anomalies are correct, but Recall at 0.34 indicates that most of the anomalies were not identified. The suitable Log-Likelihood range shows a small gap between the classes, which explains the low Recall score. Models 2 and 3 show ideal Precision values (1.0), but Recall for Model 2 remains unchanged (0.34), while Recall increases to 0.67 for Model 3. This indicates an improvement in anomaly detection while maintaining accuracy. It is worth noting that Model 3 has a significantly lower minimum Log-Likelihood value for class y=0 than Model 2, which contributes to better anomaly classification. Model 4

maintains the results of Model 3 for Precision and Recall, but has an even lower minimum Log-Likelihood value for class y=0, which may indicate an improved ability of the model to separate classes. Model 5 shows the best results with Precision and Recall at 1, which means that all the model's predictions were correct and all anomalies were detected. It is important to note that this model has a lower Log-Likelihood value for class y=1 than the previous models, which contributed to its high accuracy.

The analysis shows that the key factors for successful modeling are the optimal choice of parameters to ensure the maximum gap between the Log-Likelihood values for the classes. Model 5 is the best, but its behavior should be further assessed on a larger data sample.

Table 2: Simulation results.

Model	Precision/	Normalized Log-Likelihood
	Recall	(min(y=0) / max(y=1))
1	0.8 / 0.34	0.12 / 0.15
2	1 /0.34	0.13 / 0.15
3	1 / 0.67	0.06 / 0.15
4	1 / 0.67	-0.14 / 0.01
5	1 / 1	0.17 / 0.05

Figure 4a shows a scatter plot with normalized probabilities based on two principal components (PCA), showing how normal and abnormal points are classified based on the GMM method. Normal points are preferentially located in the same region of the principal component space, and their probabilities (estimates based on the GMM) are normalized and represented by a color scale. Abnormal points have significantly lower log-probability values. corresponding to their separation from normal points. They differ from normal points in the principal components, indicating their deviation from the expected behavior.

Figure 4b shows the histogram of the loglikelihood distribution for the two classes. Normal points have log-likelihood values between 0 and -5, with most values concentrated near values close to zero (indicating a high probability of belonging to the normal class). Abnormal points have significantly lower log-likelihood values, confirming their deviation from normal behavior. This distribution clearly shows that the model separates abnormal points from normal ones, since their log-likelihoods are very different.

Figure 4c shows the test results, which are the loglikelihoods for each point for two classes: y=0 (normal) and y = 1 (abnormal). For the y = 0 class,

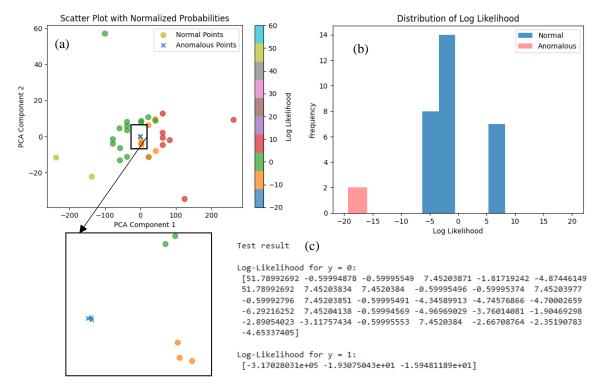


Figure 4: Simulation results for Model 5 on test data: (a) Scatter plot with log-likelihoods; (b) Log-likelihood distribution (nearest scale); (c) Test results.

the log-likelihood values range from -6 to 0. This indicates that normal points have probability values that are not very low, which correlates with a high probability of their belonging to the normal category. For the y = 1 class, the log-likelihood value is significantly lower, indicating that these points have a low probability of being part of the normal population, confirming their abnormality.

5 STRATEGY FOR DEFECT REDUCTION

Based on the constructed model for predicting defects in bakery products, a control strategy is developed that, by changing the set values of the oven temperature and humidity regulators, allows reducing the amount of defects (Fig. 5). The developed model based on the current values of the input data \overline{x} (control variables u_1, u_2 and disturbance variables z_1, \dots, z_9), before the baking stage, provides the state of the original product (not defective/defective) and if y=1 is predicted, then the control variables u_1, u_2 are corrected. If such values are not found, then a message is generated about the need for changes at the previous stages of the technological process. In particular, at the stages of dough preparation and baking by changing the process mode variables z_5, z_6, z_7 and z_8, z_9 , respectively.

The correction of the control variables u_1, u_2 can be implemented through various approaches depending on the available resources. One option is to use historical data to find cases with similar values of the disturbance variables $z_1, ..., z_9$, where y=0 was predicted, and apply the corresponding values of u_1, u_2 for correction according to the nearest neighbor principle. Another approach is to build a regression model studying the relationship between u_1, u_2 and the disturbance variables at y=0, and use this model to predict the optimal values of the control variables. Numerical optimization can also be used to find the values of u_1, u_2 that minimize the risk of defects by modeling and selecting the control variables.

Another approach is to use inverse modeling based on an existing GMM, where feasible values of u_1, u_2 are selected by gradually varying the input variables until the forecast y=0 is achieved. Alternatively, iterative simulation can be performed using the main model, gradually changing the value of u_1, u_2 until the forecast y=0 is achieved. Heuristic rules developed based on expert experience or data analysis can be effective, especially in complex or dynamic settings.

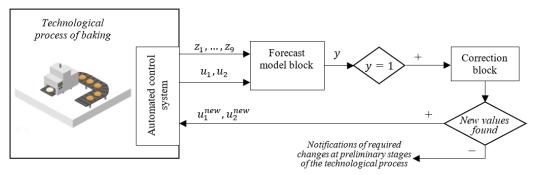


Figure 5: Structural diagram of the baking process correction strategy.

The application of both approaches – defect prediction and control variable correction – is carried out through an integrated system that can operate in real time. Machine learning models predict the probability of defects based on current values of process parameters, and the correction system changes the baking conditions to minimize defects.

6 CONCLUSIONS

As a result of the conducted research, a model for predicting defects in bakery products was developed, which uses a set of input variables to predict the probability of defects at different stages of the technological process. The accuracy of the model was 1.0 for Precision and Recall, which confirms the correctness of all defect predictions and the absence of missed defects, and the model is able to correctly identify all defective products. In terms of Log-Likelihood, the largest difference between the two classes is obtained, indicating a high probability of accurate predictions for both classes and confirming the adequacy of the model. Therefore, given the results obtained, Model 5 is the most effective in predicting defects, able to correctly classify both missing and defective products, making it suitable for application in manufacturing process conditions to reduce defects.

The model is part of a system that allows for the correction of control variables, such as oven temperature and humidity, based on current process disturbance data. Predicting defects and optimizing control variables help reduce the amount of defective products and ensure the stability of bakery product quality. The paper also considered various approaches to correcting control variables, in particular, numerical optimization methods, heuristic rules, and the use of nearest neighbor search algorithms to predict and correct values based on historical data. Thus, the proposed management strategy is an effective tool for improving product quality and optimizing the technological process in bakeries. The results of the study can be useful for implementation in industrial conditions in order to minimize defects and ensure high quality of the final product.

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