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Predicting the moisture content of organic wheat in the first stage of tempering

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Abstract: The tempering process is a key process in wheat flour milling that requires proper adjustments to achieve a desired level of flour quality and yield. The present study aims to develop a tool to predict the moisture content of organic wheat at the end of the first stage of tempering. A study case was conducted at a mill located in the Quebec region to build and compare four models: ordinary least squares (OLS), LASSO, RIDGE and ElasticNet. The models are based on wheat properties (initial wheat moisture content, wheat protein content and wheat temperature), process parameters (targeted wheat moisture content, wheat flow rate, water flow rate, wheat quantity and resting time) and tempering conditions (water quantity and day weather). The increase of wheat moisture achieved during the first tempering stage varies between 0% and 5%. The results indicated that ElasticNet model outperformed others in determining the final increase of wheat moisture with an average prediction errors of 0.21%.

Keywords: Industry 4.0, organic grains, prediction, conditioning, regression

1. INTRODUCTION

In flour production, milling is at the heart of the production system. The goal of the process is to break the grains into particles and reduce those particles into flour. Conditioning the wheat grains plays a major role in the efficiency of the process. The entire transformation process is mainly linear, composed of several steps in this order (IAOM, 2018): cleaning, conditioning and milling. First, the cleaning process has as its objective to get rid of all impurities or foreign materials that could damage machines or impact flour quality. Second, the conditioning or tempering of wheat grains seeks to increase the moisture content of the wheat grains. By increasing the moisture content to a certain percentage, the milling operations run more smoothly and efficiently (IAOM, 2018). Lastly, milling occurs and can be divided into two operations (Campbell, 2007): breaking the grains into particles and reducing the particle size. Those two operations are conducted successively in a multi-stage environment.

The organic food market is growing rapidly. Consumers are increasingly more conscious of the quality, safety and freshness of the food they buy (Rana and Paul, 2017). They are also more concerned by environmental impacts of their shopping decision. In 2019, organic food and drink sales reached more than 106 billion euros (Willer et al., 2021), an increase of 11.5% compared to 2018's sales (Willer et al., 2020). Organic flour produced from organic cereals is no exception.

Even though wheat milling follows the same process as any kind of flour production, organic flour production methods differ in some aspects from those of conventional flour. In conventional flour production, volumes are significantly greater, and a smaller variety of wheat is realized. Moreover, to improve the flour quality, chemical agents can be added to the flour (Haros et al., 2002). In contrast organic flour is produced from organic wheat, and only natural ingredients explicitly authorized by organic norms in certain proportions may be used. For those reasons, only two levers of action are possible to improve and reach the flour quality desired: wheat mixing and adjustment of the production parameters. Wheat mixing occurs at the beginning of a production run. In a previous article, we studied wheat mixing and the wheat recipe used to predict the class of the flour quality produced at the end of milling (Parrenin et al., 2021). The prediction model based on a classification tree showed mixed results for certain classes of flour quality. The results obtained by the model could be explained by a lack of information from the production system where the cleaning, tempering and milling are happening. Depending on the parameters adjusted during a production run, the flour quality is impacted.

The general objective of the research is to optimize the milling process to maximize flour production yield and deliver at the same time a desired flour quality. In this context, this article will focus on the tempering process.

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In wheat milling, several authors showed the importance of the tempering process. For example, (Fang and Campbell, 2003) show advantages of a control tempering: improved flour production yield, reduced energy consumed by the roller mills and improved profitability of the mill. But we did not find research focused on the control of the tempering process. Wheat grains are a living material with intrinsic properties that vary due to crop rotation, varieties, weather condition and crop location. Each batch of wheat grain varies in its water absorption depending on its intrinsic properties. For this reason, the tempering parameters should be adapted according to the quality of the wheat grains to reach a level of moisture content suitable for the production of a specific type of flour.

In this present article, we present a tool, based on a regression model for predicting the moisture content of organic wheat after the first stage of tempering. The model will provide insight into which variables have the greatest influence and impact on the tempering process and will offer a decision support tool for adjusting the parameters used during the first stage of tempering.

Literature review is presented in Section 2. Section 3 explains the method followed to build and develop the tool presented in this study. Finally, Section 4 demonstrates the tool applicability in a wheat milling plant.

2. LITERATURE REVIEW

Tempering represents a key stage in the wheat milling process. It conditions the wheat for the milling process. Although few studies have shown the importance of the tempering process, it remains difficult to control and automate.

2.1 Tempering process

Tempering is the process whereby water is added to wheat grains, followed by a period of resting in an empty silo to let the water penetrate in the wheat (IAOM, 2018). Studies have measured the impact of the tempering process on flour quality and flour yield (Cappelli et al., 2020; Doblado-Maldonado et al., 2013; Hook et al., 1982; Kweon et al., 2009; Warechowska et al., 2016). Depending on the wheat moisture content attained, flour yield and flour quality are impacted during the milling process. As the wheat moisture content increases, yield output decreases and flour quality increases (Kweon et al., 2009; Warechowska et al., 2016). A good trade-off has then to be found, in particular for the manufacture of white flour, which should not be contaminated by the bran.

Wheat moisture is a key indicator for good storage. (Campbell, 2007) explains that wheat can be stored almost indefinitely if its moisture content is kept below approximately 14%. However, before milling, it is suggested to raise the wheat moisture to about 16% (Campbell, 2007). This increase has the effect of hardening the bran while making the endosperm more friable. In producing white flour, the goal is to extract as much endosperm as possible from the grain without any bran contamination. Tempering thus helps during milling to separate the endosperm from the bran, which by consequence improves the final flour quality. Moreover, tempering helps compensate the loss of moisture that occurs during milling operations. As flour prices are fixed according to quality and weight, there is an economic interest to increase the final flour moisture content.

However, adjusting the tempering process is difficult as it is affected by several factors. According to (IAOM, 2018; Kweon et al., 2009) those factors include: wheat properties, moisture, temperature, time and the tempering bin space available. Furthermore, the wheat mixes realized before the tempering stage add complexity to the good control of the process.

During the tempering stages, the miller, by his experience and knowledge, adjusts tempering parameters depending on the wheat quality, wheat mixes and environmental conditions. Depending on the type and quality of flour desired, a target moisture content is established, representing the moisture content to be reached at the end of the first tempering stage. This target moisture content (Ht) with the flow of the wheat grains (Fwg) and the initial moisture content of the wheat (Hi) will determine the flow of water (Fw) used during the tempering process. It is calculated by formula 1 (IAOM, 2018):

$$Fw(L/h) = \frac{(Ht - Hi)Fwg}{100 - Ht} \tag{1}$$

Other parameters controlled by the miller are the flow of wheat grains, wheat quantity, the duration of the resting time and the number of tempering stages.

2.2 Prediction methods in manufacturing processes

Nowadays, manufacturing processes collect vast quantities of data. Analyzing this data can help uncover hidden patterns and knowledge (Ge et al., 2017). Depending on the data at hand and the objective, different techniques can be applied. For example, statistical tools such as PLS (Partial Least Squares) and regression models are useful for understanding the relationships between variables as well as to learn the variables of interest. Statistical tools and regression models have been applied, for example, to study the process setting and attributes of dairy product manufactured (Roupas, 2008; Poveda et al., 2004), as well as in the bioethanol production environment for predicting the ethanol yield production from process parameters (Maiti et al., 2011).

Organic flours are made from organic cereals. The cereals are a living raw material which gives the wheat unique intrinsic properties. In this context, the objective will be to use statistical tools or regression analysis to bring a better control to the tempering parameters.

3. METHOD

The proposed tool will be based on a regression model. To build and train the model, a few steps will be followed. Figure 1 shows the method used with its different steps.

First, the data is collected. Second, it is formatted, cleaned and transformed to make it ready for a regression model. Third, the model is trained. Lastly, validation measures the performance of the model on new data. A comparison

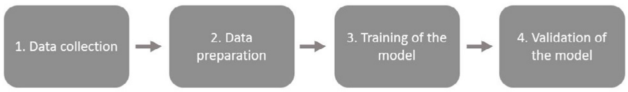

Fig. 1. Method

of the performance of the different regression models will be presented. To our knowledge, no predictive model applied to grains tempering exists in the literature review that could be compared to.

3.1 Data collection

(Parrenin et al., 2020) conducted an analysis and an overview of the flour manufacturing process, including the logistic and the operation processes. The processes were represented on a cartography, which made it possible to identify checkpoints along the value chain and the data collected at those checkpoints. A good comprehension of the workflow and the system is essential to determine the data to be used. Depending on the IT infrastructure and software used on the shop floor, different methods allow to collect the data. For equipment or databases connected to the IT infrastructure, it is possible to query the data directly from the architecture (with SQL queries or REST APIs), otherwise back ups of the isolated data are necessary.

3.2 Data preparation

Most of the time, the data collected is not ready to be used and analyzed directly. For this reason, it is formatted, cleaned and transformed. Inconsistent data can be found during the formatting of the data. Statistical tool analysis or machine learning algorithms are helpful to detect outliers present in the dataset (Ahmed and Mahmood, 2013; Escalante, 2005). With the help of clustering techniques, it is possible to spot outliers and check the real causes of the existence of the outliers. By verifying their information inputs, corrections can be made. This implies deleting the example if the data doesn't make sense, correcting it if possible or keeping it as it is if there are no incoherences in the example. Also, different approaches can be used to deal with missing values (Burkov, 2019): removing the examples, using learning algorithms that handle missing values and using data imputation techniques. Data imputation consists of filling in partially missing data with substituted values (Lakshminarayan et al., 1999). Then, the cleaned data must be transformed to the right format to process it in a machine learning model efficiently. If independent variables have vastly different scale sizes and the machine learning algorithm is sensible to those different scales, it is recommended to apply feature scaling on the data (Burkov, 2019).

Finally, all the data is merged in one table. Each row represents an example of the first tempering stage run. Each column represents a feature variable. The last column holds the output variable that has to be predicted. To train and evaluate afterwards the learning algorithms, the prepared data is split to two datasets where 85% of the dataset is used for training the model and 15% is used for testing the model.

3.3 Training of the model

After the data has been prepared, we select and train a model to predict the output variable. In the present case, a regression model is well suited for the purpose. Deep learning models such as neural networks have not been considered for a regression model due to the small size of the dataset available. Different regression models exists: linear regression, polynomial regression, stepwise regression, ridge regression and elasticnet regression. Each one has some advantages, depending on the data at hand and the hyperparameters to adjust. For these reasons, several models will be built, optimized if possible and compared.

In a regression model, in the presence of multiple independent variables, it is essential to check for multicollinearity. Multicollinearity happens when independent variables are highly correlated to each other (James et al., 2013). It can cause the model to overfit and impact the model performance. To detect multicollinearity, several options are possible. First, a correlation matrix would provide a good indication on the possible existence of multicollinearity between pairs of independent variables. Second, the Variance Inflation Factor (VIF) test can be conducted. In general, multicolinearity exists and becomes problematic when a VIF value greater than 10 is obtained (James et al., 2013). In the case of multicollinearity, it is possible to delete or transform the dependent variables. Another way to treat this issue is by using regression algorithms such as LASSO, RIDGE and ElasticNet that can reduce the risk of multicollinearity. By adjusting their different parameters, it is possible to penalize some independent variables and reduce or eliminate their influence on the model. The main difference between LASSO, RIDGE and ElasticNet is the penalty terms they use for the different weights present in the model (Burkov, 2019).

To evaluate and tune the hyper-parameters of regression algorithms, k-fold cross-validation can be used (James et al., 2013). The k-fold cross-validation splits the dataset into k-folds. In an iterative process, each of the k-folds will be used to test the model and the rest will be used to train the model. The average of the prediction accuracy on each k-fold represents the model performance. By testing different values of hyper-parameters and evaluating the model performance, we can find the best hyper-parameters that generalize the model.

3.4 Validation

To evaluate the pertinence and performance of the model, a validation step is required. The validation of the model is conducted on the test set. The metrics used to evaluate the performance of the model will be based on the R-square and Mean Square Error (MSE). The R-square calculates the degree of variation explained by the model (James et al., 2013). It is a metric that fluctuates between 0 and 1. A value close to 1 indicates that the model explains most of the variation of the data, thus making the model accurate for future prediction. Finally, MSE measures the average error of the predicted values from the model compared to the real values (James et al., 2013). A small MSE indicates low distant average errors between the regression model and the real values, which implies an accurate model for making future predictions. The threshold to define a good MSE score from a less acceptable score will vary according to individual needs and the scale used from the output variable.

4. METHOD APPLICATION

This method is tested on a case study to predict the increase of wheat moisture achieved during the first tempering stage in a flour production context. The context is introduced and then the approach, following the same steps described in Section 3, is detailed. Finally, the results are presented and discussed.

4.1 Context

The case study takes place in a wheat milling environment in cooperation with an industrial partner named "La Milanaise". La Milanaise is specialized in the transformation of organic cereals into organic flour. The company, a small and medium sized enterprise (SME), is facing a large increase in demand for organic flour. This growth has become even more pronounced during the recent covid-19 pandemic. To increase the production flow and have better control over the quality output, the tempering process is investigated. Depending on the quality of the grains, their variety, the environmental conditions and the type of flour expected, different setups are required during the tempering process. At the mill, the tempering process can take place in up to three stages. We will focus on the first stage, which is always done except in rare cases where the wheat moisture level is high (above 16%). The adjustment of the tempering parameters is currently done based on professional expertise and experience, which is difficult to capture and share. A decision support tool will be useful in this context.

This mill lies in a specific context different from mills based in other regions of the globe (e.g., Europe, North Africa or the United-States). The mill from our case study is located in the Quebec region where the temperature fluctuates highly throughout the year, from -32 degrees Celsius during the coldest days to 36 degrees Celsius during the warmest days (Gouvernment of Canada, 2021). This fluctuation impacts the tempering process.

4.2 Method application in wheat mill

Data collection

As with most SMEs, the data at La Milanaise is quite dispersed among the company's machines and various Excel files and databases. Most data available from the sensor equipment of the mill is stored in an SQL Server database linked to the Supervisory Control and Data Acquisition (SCADA). The data is recorded at regular intervals, every 10 minutes. The information includes essentially the quantity of wheat transferred from one stage to another and the quantity of water used. From that information it is possible to calculate the resting time in each stage of the tempering process.

The analysis of the wheat quality and control parameters of the tempering stage are stored in Excel files. For each production run, an Excel file is created that contains information about the quantity of wheat used, the different tempering stage conditions and parameters adjusted as well as the milling conditions. The milling conditions will not be used in this present study as the focus is toward tempering.

To efficiently collect the data stored in Excel files, a Python program has been used. As the Excel files follow an identical template, the Python program opens each file, collects the information from specific cells and stores it in a table. The table is saved in a CSV file, which will make data processing easier.

To get a better sense of the data, we will define and distinguish the variables that require adjustments from those that do not. The adjustable variables for the tempering process include: *the target wheat moisture content*, *wheat flow rate*, *water flow rate*, *wheat quantity* and the *resting time* for the wheat grain. The non-adjustable variables include: *initial wheat moisture content*, *wheat protein content*, *wheat temperature* and *water quantity*.

Data preparation

The data collected has many flaws. First, regarding the SCADA database, the tables store a lot of null values translating as a non-movement of the wheat grains between the different stages. These lines are deleted. Then, regarding the Excel files, some information is missing or incoherent. The missing information is filled by collecting additional information from other sources of data. If other sources of data are unavailable to complete the information, the examples that contain missing information are deleted.

To explore the data, we will focus on one mix of wheat category. Different categories of wheat have been created by La Milanaise to distinguish them from their hardness index. The hardness index will influence the level of water absorption of wheat grains. By selecting one mix of wheat category, this will restrict our data to 266 examples out of the 873 available. Without any missing values, we can start analyzing the data. Table 1 presents the VIF test calculated from the different features.

Table 1. Variance inflation factor test

Feature	VIF
Day	6.17
Initial wheat moisture content	9842.31
Target wheat moisture content	11648.94
Wheat flow rate	537.20
Water flow rate	563.05
Wheat quantity	42.9
Resting time	2.34
Wheat protein content	335.22
Wheat temperature	12.89
Water quantity	31.17

From Table 1, we can see high VIF values, which suggest a high presence of multicollinearity between the features. To reduce it, we transform and combine two features. We calculated a new feature called *moisture content increase target* by applying the difference between the initial and the target of the wheat moisture content. It measures the percentage of humidity we want to add to the wheat grain. In other cases, we delete the features. To delete the non-useful features, regression algorithms are explored to identify the relevant variables for predicting the final wheat moisture increase.

To visualize the data, we plot the different variables. Figure 2 shows a pair plot between two features and the output variable which corresponds to the final wheat moisture increase realised at the first tempering stage.

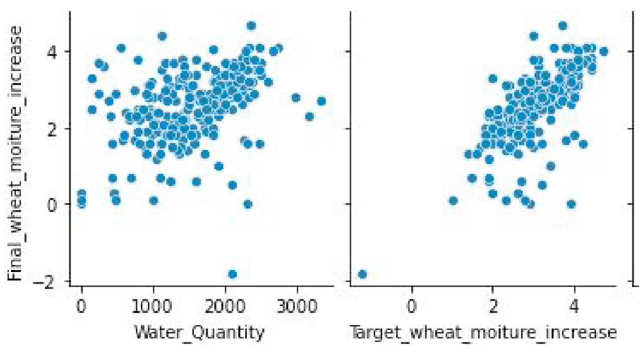

Fig. 2. Pair plot

In Figure 2, the first graph on the left explains the quantity of water used in relation to the increase in wheat moisture content realized. It is interesting to note that sometimes the use of only a little amount of water leads to a high increase of the wheat moisture content. Sometimes, the opposite happens. We can easily spot some incoherent values or values that need to be investigated. Negative values are corrected if possible and deleted otherwise. Those examples need to be investigated. The second graph from the left highlights a linear relationship between the target wheat moisture increase, which controls the flow of water, and the final wheat moisture increase.

For better outlier detection, the DBSCAN algorithm is used. We first scale the data by standardizing the features. A 3D graph is then created with x-axes showing the target fixed by the miller for the first tempering stage, y-axes showing the final or real increase of the wheat moisture content and z-axes showing the number of hours allocated for the resting time of the wheat kernel in the silo. The shape of the data points represents the season period of the tempering stage.

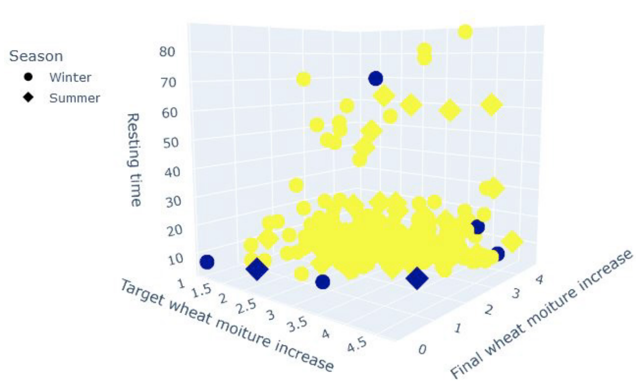

Fig. 3. DBSCAN plot

Figure 3 shows seven potential outliers. They are checked and corrected if necessary or deleted if they are incoherent. Finally, statistical analysis and DBSCAN lead to nine examples being removed from the 266 examples available.

Training of the model

We select the most popular wheat mixes, which gives us 257 examples remaining. 85% of the data is selected to train and fit the model, while the other 15% will constitute the test set. As explained earlier, we train several models using Linear Regression, LASSO, RIDGE and ElasticNet. As some features are surely more important than others, the different models will be able to fix the best coefficient for each feature. The output variable (Y) is the increase in the moisture content of wheat grains. The scale of the output variable varies from 0% to 5%. This means that, from the data, no wheat grains increased their moisture content by more than 5% during the first tempering stage. For each model, a resampling method was used to adjust the different existing parameters of the different models. For that, we used a k-fold cross-validation, setting k equal to 5.

Validation of the model

All models are validated on the test set with R-square and MSE.

4.3 Results

Figure 4 compares the performance of the different models. This figure compares the R-square and MSE metrics of the different models.

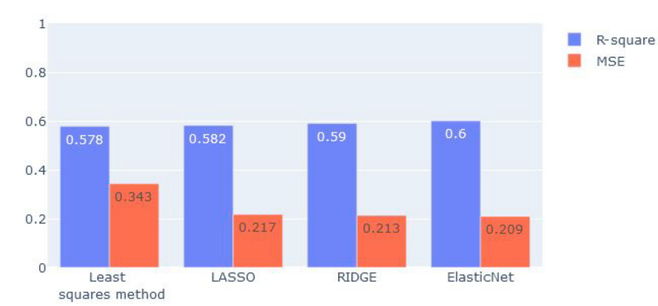

Fig. 4. Model performance

Figure 4 shows that the best model is ElasticNet. It gets the highest R-square score and the smallest MSE value. The different regression models have approximately the same R-square score, but LASSO, RIDGE and ElasticNet models offer lower average errors in terms of prediction.

In the ElasticNet model, seven variables are considered: water quantity (X1), initial wheat moisture content (X2), target wheat moisture increase (X3), wheat temperature (X4), water flow (X5), wheat quantity (X6) and resting time (X7). The regression model is the following:

$$\begin{aligned} Y = 2.64 + 0.15(X1) - 0.16(X2) + 0.33(X3) \\ + 0.04(X4) + 0.06(X5) - 0.13(X6) + 0.04(X7) \end{aligned} \quad (2)$$

Four variables have a high impact on the increase of the moisture content (Y): the target wheat moisture increase (X3), the initial wheat moisture content (X2), the water quantity (X1) and the wheat quantity (X6).

The mean square error for the model is around 0.21%. This result is quite low and accurate enough for adjusting the tempering parameter to increase adequately the moisture content of the wheat grains. However, the MSE does not indicate how high an error prediction can be from the real value. As we would like to calculate the model uncertainty and know the accuracy of the future prediction, it is best to calculate the prediction intervals. Given a Gaussian distribution and a significance level of 95%, we find an interval equal to 0.92. This result means that there will be 95% probability that the future real value is between +/- 0.92% of the predicted value from the model. As most values from the moisture content increase are between 0% and 5%, this prediction interval is high and needs to be improved to ensure a more reliable model.

5. CONCLUSION

In this study, four different regression models have been developed and compared to determine the final wheat moisture content at the end of the first tempering stage. The models are based on wheat properties, tempering conditions and tempering parameters for one specific wheat mix category. The ElasticNet model offers the best performance in terms of accuracy with an average prediction error of 0.21% and an R-square of 0.6. Although the model shows good results, deeper research is needed to improve the reliability of the model by trying to reduce the prediction intervals. Further studies will be conducted to include weather data and analyze the different categories of wheat mixes. Future steps will be to analyze the milling process and understand the setup required for maximizing the yield output while producing the desired flour quality.

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