

Ensemble Learning based on Regressor Chains: A Case on Quality Prediction

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Abstract: In this study we construct a prediction model, which utilizes the production process parameters acquired from a textile machine and predicts the quality characteristics of the final yarn. Several machine learning algorithms (decision tree, multivariate adaptive regression splines and random forest) are used for prediction. An ensemble method, using the idea of regressor chains, is developed to further improve the prediction performance. Collected data is first segmented into two parts (labeled as “normal” and “unusual”) using local outlier factor method, and performance of the algorithms are tested for each segment separately. It is seen that ensemble idea proves its competence especially for the cases where the collected data is categorized as unusual. In such cases ensemble algorithm improves the prediction accuracy significantly.

1 INTRODUCTION

With the advances in communication technologies, data gathering from machines and processes at industrial plants becomes easier. Industrial internet-of-things (IIoT) revolution along with the fog computing idea, change the way data is being treated in manufacturing plants. Live data from manufacturing processes, machines and products are being collected with high resolution and executing advance analytic tasks at the industrial plant premises becomes possible. Considering the analytics efforts in the manufacturing plants, it is seen that quality prediction and predictive maintenance stand out as the most frequently addressed analytics application examples.

In this paper we focus on a quality prediction application at a textile plant, Deteks Fashion Co.Ltd. We first implement a set of well-known machine learning algorithms (decision tree, multivariate adaptive regression splines and random forest) with proven performance in quality prediction. For each model, the performance is tested by using three different quality metrics. Considering the performance of implemented machine learning algorithms, we propose an ensemble algorithm, which is based on regressor

chain idea. The most important finding of the paper is that once production is taking place different than the usual settings, prediction accuracy of the classical machine learning algorithms significantly drops for some quality metrics. For such cases, the ensemble algorithm turns out to be useful, yielding lower prediction error in two thirds of the dataset.

The rest of the paper is organized as follows. Section 2 provides brief background information on the textile manufacturing process and outlines the methodology used in the study. Section 3 presents the data and results of the numerical analysis. Final section lists the concluding remarks.

2 BACKGROUND AND METHODOLOGY

2.1 Textile Manufacturing Processes

Textile manufacturing process we chose to analyze mainly consists of three main processes: 1) warping, 2) weaving, 3) finishing. In the first stage, yarns are made suitable for weaving by passing through the winding, unraveling, sizing, weaving draft and knotting steps. In these steps, the yarns are wrapped in desired tension and order, and subjected to various operations to gain strength. In the weaving process, the

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fabrics are subjected to mouth opening, weft insertion and tufting to ensure that the warp and weft yarns intersect. In the finishing stage, which is the last stage of production, the desired color, touch and special effects are provided to the fabric. After these manufacturing stages, some samples are taken randomly from the final product to conduct various quality control tests in laboratory.

In this work, we concentrate on the finishing process and integrate our algorithm into the production process of the finishing machine such that production parameters and information from the incoming fabric constitute the input for the algorithm; and the quality data (output) of the process is obtained from conducted laboratory tests. Collected input and outputs are matched with each other by using time mapping scenarios, in which time tags in the database is taken into account. The input data is collected through data collection devices (i.e. gateways) and programmable logic controller (PLC) of the finishing machine. The general flowchart of proposed methodology is presented in Figure 1.

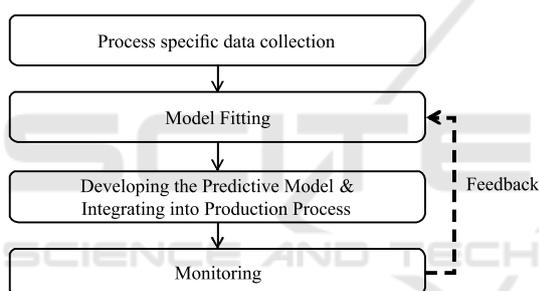


Figure 1: Framework of the proposed method.

As can be seen in Figure 1, after process specific data is collected, a model fitting phase is executed. Details of the selected models are presented in the next subsections. We first present the multi-target regression and regression chain idea, then list the predictive models used in the study. After model fitting, the selected model (or models) are integrated into PLC and production is started to be monitored with live quality predictions. A natural next step is integrating an auto-learning mode (through feedback from process data), which enables re-learning of the model parameters in the course of the production, without manual intervention.

2.2 Multi-Target Regression

Multi-Target Regression (MTR) or Multi-Output Regression indicates regression models which uses a common training set (input variables) to predict multiple targets (output variables). In a literature survey about MTR methods by (Borchani et al., 2015),

there are mainly two ideas behind the MTR methods in literature: transforming multi-target problems into single-target (ST) problems, then applying traditional regression models and concatenating the results such as Multi-Target Regressor Stacking (MTS) (Spyromitros-Xioufis et al., 2012), Regressor Chains (RC) (Spyromitros-Xioufis et al., 2012) and Multi-Output SVR (MO-SVR) (Zhang et al., 2012); or using algorithm adaptation methods which have the ability to capture internal relationships between the target variables, such as Churds and Whey method (Similä and Tikka, 2007), Simultaneous Variable Selection (Struyf and Džeroski, 2005), Multi-Target Regression Trees (De'Ath, 2002) and extended MO-SVR (Vazquez and Walter, 2003).

According to the benchmark comparison conducted on twelve different datasets with different shapes, statistical methods fail to improve ST regression results in cases where a true and linear relationship between outputs is not verified; rather they could produce a detriment of the predictive performance (Borchani et al., 2015). On the other hand, some other algorithm adaptation methods (e.g. MO-SVR) benefit only in terms of calculation time and complexity reduction, while the regression trees method achieves improvement in predictive performance as well, compared to the ST approach. In addition to these findings, a clear inference could not be made about the benefit of problem transformation methods (MTS and RC). This is because the predictive performance of MTS and RC approaches is so sensitive in the randomization process of these approaches (e.g. due to the order of the chain) (Borchani et al., 2015).

MTS and RC methods are firstly introduced as extensions of problem transformation approaches of multi-label classification in the multi-target regression context. These two methods are basically based on the approach of training independent single-target regression models for each target variables and training a comprising model by augmenting the input space dimensions with gathered prediction results. In this paper, we are going to focus on a real-life application of RC approach and its extension Ensemble of Regressor Chains (ERC) proposed in (Spyromitros-Xioufis et al., 2012).

2.2.1 Regressor Chains and Ensemble of Regressor Chains

RC is inspired by the Classifier Chains method and the main idea behind it is chaining single-target models. RC is based on building of regression models for each target variable by sequentially training the targets in order of a randomly determined chain. For the first target variable selected within the specified se-

quence of the chain, the regression model is trained independently of the other target variables, and the predicted target values are added to the training set as a new input vector for prediction of the next target variable. The regression model of the new target variable within the chain sequence is trained with the resulting augmented input matrix and the same process is repeated for all subsequent targets in the chain.

Graphical illustration of RC is shown in Figure 2. In the illustration, there are three output (target) variables ($y_1, y_2,$ and y_3) and training input data (X). In the first stage of training process starts with fitting a model (f_1) for the first output variable (y_1) by using base inputs (X). Then, in the second stage, a new model (f_2) is fitted for the second output variable (y_2) by using modified input that is created with concatenating base inputs (X) and the actual values of the first output (y_1). Finally, f_3 is created by using the third output variable (y_3) and concatenated data ($X, y_1,$ and y_2) in the third stage.

In testing process, predictions for the first output (\hat{y}_1^q) are made by using (f_1). Then, the first predictions are added to the test input data (x_q), and it is used for predicting the second output (\hat{y}_2^q) by model (f_2). In the last step, first two predictions ($\hat{y}_1^q,$ and \hat{y}_2^q) concatenated with the test input data (x_q), and \hat{y}_3^q is predicted by model 3 (f_3).

The main problem of this method is that the randomness in determining chain sequence causes significant differences in predictive performance. In order to avoid this problem, ERC method is proposed by (Spyromitros-Xioufis et al., 2012). The ERC method suggests using a set of regression chains consisting of all possible chains or a group of chains which is randomly selected if the output dimension is too high, in an ensembled structure. After determining the set of chain sequences, the ERC approach predicts the target variable for each stage of the chain and finally presents their averages as predicted values for each target variable.

The difference between RC and ERC is that RC takes the single prediction for each output in a certain sequence. However, ERC makes predictions for all permutations of sequence and gives the final prediction as the average of all predictions for each output.

2.3 Predictive Models

MTR is a meta-learner which can use different estimators and set of learning sequences in a pre-determined configuration. In this part, we introduce three common regression techniques to conduct a benchmark test and determine the most appropriate one to apply our dataset. These estimators are: 1) De-

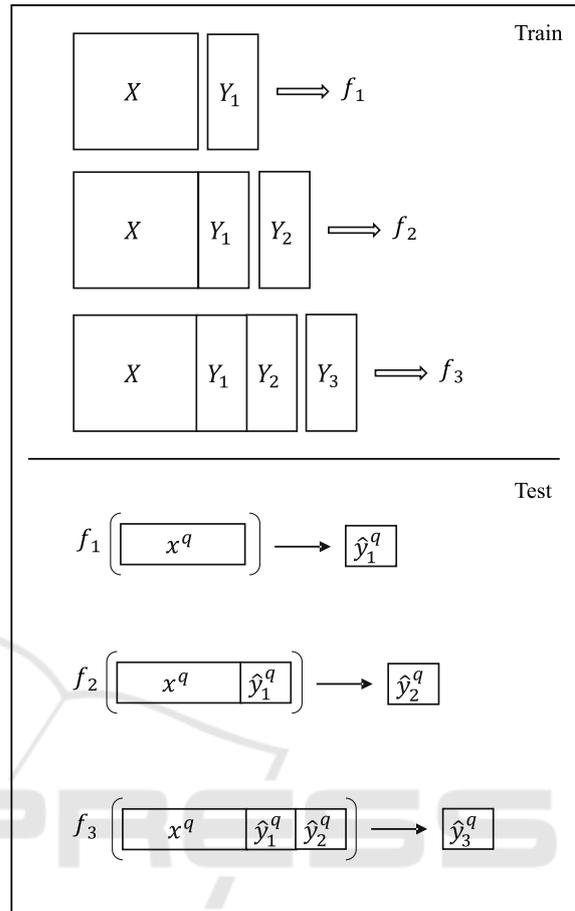


Figure 2: Graphical illustration of RC.

cision Tree Regressor, 2) Random Forest Regressor, and 3) Multivariate Adaptive Regression Splines.

2.3.1 Decision Tree Regressor

Decision Tree induction is one of the most important supervised learning methods which is used for classification and regression. Decision Tree Regressor constructs a flowchart-like structure where each internal (non-leaf) node denotes a test on an attribute, each branch corresponds to an outcome of the test, and each external (leaf) node denotes a class prediction. At each node, the algorithm chooses the “best” attribute to partition the data into individual classes (Han et al., 2011). The main idea here is to create a decision tree model that minimizes error on each leaf. Different algorithms may be applied to build decision trees such as Classification and Regression Trees (CART) which uses Gini Index as metric and Iterative Dichotomiser 3 (ID3) which uses Entropy function and Information gain as metrics (Quinlan, 1986). We used Gini method in CART algorithm.

2.3.2 Random Forest Regressor

Random Forest is an ensemble learning method that aims to improve predictive accuracy and prevent overfitting by fitting multiple decision trees on various sub-samples of the dataset and combining them under a single meta-estimator (Breiman, 2001). Random Forest Regressor (RF) uses the average prediction for regression of trees which are constructed by training on different data sample. These samples are created by Bootstrap Aggregation (or bagging).

2.3.3 Multivariate Adaptive Regression Splines

Multivariate Adaptive Regression Splines (MARS) is a non-parametric extension of the standard linear model without any assumption about the underlying functional relationship between the dependent and independent variables. MARS model is obtained by using combination of piece-wise basis functions, forward and backward passing procedures in the regression models. Each term in a MARS model is a product of so called "hinge functions". A hinge function is a function that's equal to its argument where that argument is greater than zero and is zero everywhere else (Friedman et al., 1991).

MARS builds a model which is formed followingly:

$$f(x) = \sum_{i=0}^k c_i B_i(x_i), \tag{1}$$

where \mathbf{x} is a vector of sample features, B_i is a piece-wise function that consists of a set of basis functions and c_i the coefficient. Basis function may behave in three different ways based on the input range: First, it can be constant 1, to reduce bias. Second, it can be a hinge function $h(x) = \max(0, x - t)$ or $\max(0, t - x)$, where t is a constant, so the model represents nonlinearities. Third, it can be a product of multiple hinge functions to combine interactions between features.

3 EXPERIMENTAL SETUP

3.1 Dataset

In this study, we apply the algorithms to dataset obtained from paired process data (signals) of textile manufacturing. There are total of 1,511 rows, one row for each lab sample in dataset, and each lab sample has 19 signal values, such that weaving speed, temperature, and yarn tension, as input for algorithms; and 3 quality metrics, water permeability (Metric 1),

tear strength (Metric 2), and abrasion resistance (Metric 3), that are obtained after lab sample assessed in the laboratory as output of algorithms.

The statistical summary of the 19 features is shown in Table 1. Also, the Z-normalization of target metrics 1, 2 and 3 is given in Figure 3.

Table 1: Feature Summary Statistics.

Feature	Mean	Std	CoV*	Min	Max
0	70.0	1.0	0.0	65.7	74.5
1	-10.8	1.2	-0.1	-14.5	-7.7
2	-4.2	1.2	-0.3	-8.5	-2.2
3	-0.2	0.1	-0.3	-0.4	0.0
4	-0.3	0.2	-0.5	-0.3	0.0
5	7.4	2.1	0.3	0.0	14.8
6	31.9	2.6	0.1	28.5	53.7
7	302.9	77.1	0.3	198.9	401.4
8	27.2	0.0	0.0	27.2	27.2
9	37.9	0.0	0.0	37.9	37.9
10	25.2	2.8	0.1	20.3	31.8
11	49.9	4.1	0.1	42.3	57.3
12	63.0	6.9	0.1	44.4	70.4
13	28.3	1.6	0.1	23.2	32.3
14	25.3	2.2	0.1	18.8	31.8
15	152.6	4.9	0.0	143.4	163.7
16	146.5	8.8	0.1	119.1	154.6
17	225.8	0.6	0.0	225.1	226.3
18	20.7	1.5	0.1	17.7	25.2

*CoV: Coefficient of Variation

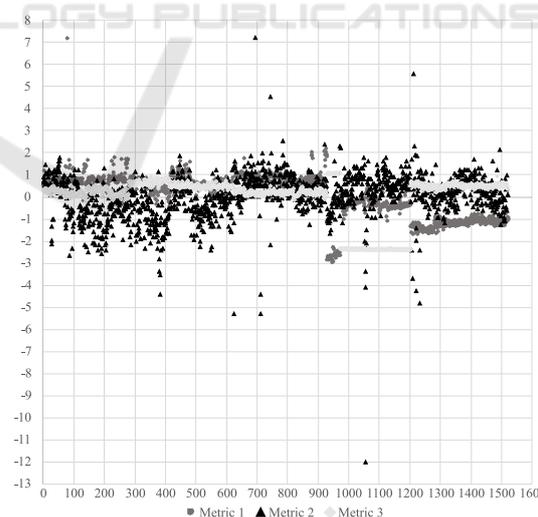


Figure 3: Distribution of Target Data.

After examining the target data, it is observed that the variance of Z-values of Metric 2 is much higher than that of other metrics. Feature importance analysis is performed for each metric to see whether the characteristics of Metric 3 shows similarities in terms of ability to be expressed by features. Analysis results

can be seen in Figure 4, 5 and 6.

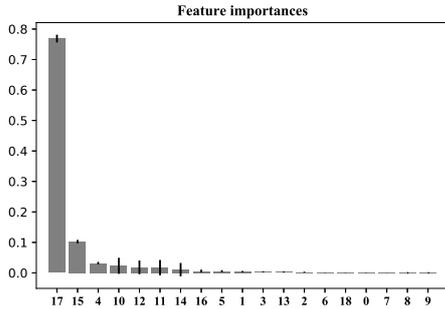


Figure 4: Feature Importance of Metric 1.

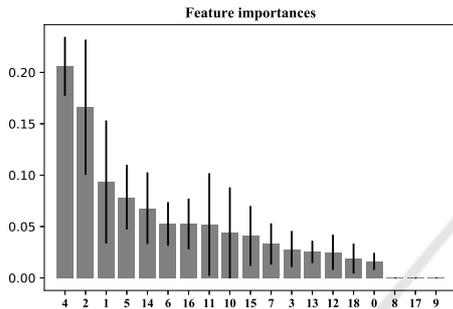


Figure 5: Feature Importance of Metric 2.

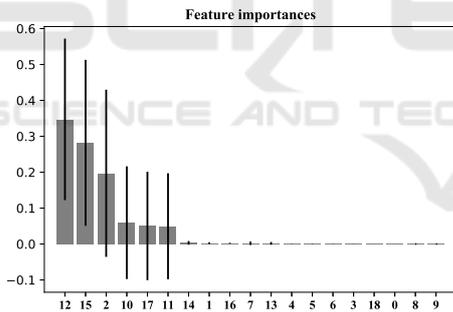


Figure 6: Feature Importance of Metric 3.

According to the feature importance analysis, while there are at least one features have minimum of 20% importance on Metric 1 and 3, the importance rate of all features are less than 20% for Metric 2. In this sense, it can be concluded that Metric 2 is disadvantageous compared to other metrics in terms of both the distribution character and the power to be expressed by existing feature set.

3.2 Outlier Detection

In order to obtain the most suitable models for the natural characteristics of production process, the data is divided into clusters according to the Local Outlier Factor (LOF) method (Breunig et al., 2000). For any

given data instance, the LOF score is equal to ratio of average local density of the k -nearest neighbors of the instance and the local density of the data instance itself (Chandola et al., 2009). The local density of each sample is compared with the local densities of the neighbors and the samples with significantly lower density than their neighbors are specified as outliers. In this study, the number of neighbors, k , is assumed as 10, and the cluster which has greatest dissimilarity is extracted and labeled as “unusual”. Segmentation yields two segments of size 1,431 (“normal” segment) and 80 (“unusual” segment). We divide the “normal” dataset further into training and testing sets, which have 1,144 and 287 data points respectively.

In the next section, we use several machine learning algorithms and compare their prediction performance using a series of statistical analysis. The analysis conducted in two major steps. First, analysis regarding the “normal” data is presented. Then, the analysis for the “unusual” data is presented, where it is seen that the ensemble of regressor chains significantly outperforms the single target model.

3.3 Implementation and Analysis

In the first step of the numerical analysis, single-target regression models are created for each metric in the “normal” dataset. Then, the best performing single-target regression model is selected to be compared with the ERC model. During the comparisons, we use MAPE as the key performance metric and conduct a set of statistical tests/analysis, which are vector comparison, paired t -test and one-way ANOVA test. In the second step, similar comparison between single-target regression model and ERC is conducted using the “unusual” dataset.

For the sake of completeness, we present the details of the metrics, statistical tests and analysis we use during the comparison.

In paired t -test, the mean of the observed values for a variable from two dependent samples are paired and compared. As we use different algorithms to predict the same set of data points, pairing is direct possible as a natural consequence of the process. The test is used to decide whether the sample means compared are identical or not. The differences between all pairs are calculated by the following equation:

$$t = \frac{\bar{X}_D - \mu_0}{\frac{s_D}{\sqrt{n}}}, \quad (2)$$

where \bar{X}_D and s_D are the mean and standard deviation of those differences, respectively. The constant μ_0 equals to zero if the underlying hypothesis assumes the two samples are coming from populations with identical means, and n represents the number of pairs.

The one-way ANOVA test compares whether mean of two or more samples are the same. The main assumptions of ANOVA test is that the distribution of each sample is normal and the samples are independent.

In vector comparison analysis, algorithms are scored for their prediction performance for each and every data point separately. The algorithm yielding the minimum absolute percentage error for the given data point receives 1 (winner), others receive 0. Test results for MAPE comparison, vector comparison and *t*-test comparison are given in Table 2, Table 3, Table 4 and Table 5 respectively. In Table 2, test and (train) errors are given respectively.

Table 2: MAPE Comparison for ST Models.

	RF	DTR	MARS
Metric 1	0.020 (0.011)	0.023 (0.017)	0.027 (0.024)
Metric 2	0.045 (0.030)	0.046 (0.044)	0.047 (0.046)
Metric 3	0.003 (0.002)	0.030 (0.030)	0.007 (0.007)

Table 3: Vector Comparison.

	RF	DTR	MARS
Metric 1	126	78	83
Metric 2	95	104	88
Metric 3	132	107	48

Table 4: Paired *t*-test Comparison.

	$y - \hat{y}_{RF}$	$y - \hat{y}_{DTR}$	$y - \hat{y}_{MARS}$
Metric 1	0.818	0.694	0.914
Metric 2	0.621	0.459	0.536
Metric 3	0.982	0.398	0.275

Table 5: One-way ANOVA Comparison.

	p-value
Metric 1	0.935
Metric 2	0.983
Metric 3	0.308

When the MAPE values are examined, it is observed that the values are very close to each other but the best test results are obtained by RF for three metrics. The best results for Metric 1 and Metric 3 are taken by RF in the vector comparison, whereas MARS model predicted nine lab samples better than RF for Metric 2.

Paired *t*-test results presented in Table 4 reveal that all predictions yielded residuals with zero mean. For the constant variation assumption, RF model's residual vs. fitted plot for Metric 2 is presented in

Figure 7. Figure 7 reveals that there is no indication for the violation of constant variation assumption.

Following these, analyzes it is determined that working with RF would be more appropriate for this dataset and it is chosen as the baseline model.

The noteworthy point here is that the MAPE value of Metric 2 is higher than MAPE values of other two variables. In order to better understand the relationship between outputs, correlation between the output values are measured and it is seen that there is no linear relationship between the output of Metrics 1-2 and 2-3 as shown in Table 6.

Table 6: Correlation Matrix of Output Variables.

	Metric 1	Metric 2	Metric 3
Metric 1	1	-0.019	0.018
Metric 2	-0.019	1	-0.200
Metric 3	0.018	-0.200	1

At this point, multi-output regression approach can be seen as an opportunity to improve the relatively bad performance we observe for Metric 2. With the regressor chains method, all input and output variables can be evaluated together, thus the dependencies and internal relationships between them that have a positive impact on the predictive performance may be unveiled (Borchani et al., 2015). Since we have small number of outputs, regression models are trained for all possible chain sequences by applying the ERC framework, and the mean of the predicted values from each model are recorded as final predictions. MAPE comparison, vector comparison and paired *t*-test results are shown in Table 7, Table 8 and Table 9.

Table 7: ERC vs ST Mape Comparison for testing.

	ERC	ST
Metric 1	0.019	0.020
Metric 2	0.042	0.045
Metric 3	0.003	0.003

Table 8: ERC vs ST Vector Comparison for testing.

	ERC	ST
Metric 1	159	129
Metric 2	150	138
Metric 3	133	155

According to Table 7, ERC approach provides %5 and %4.5 improvement over the performance of ST in predicting Metric 1 and Metric 2 respectively. The benefit of the ERC approach for Metric 1 and 2 is also obvious in the vector comparison test. For Metric 3, on the other hand, the number of predictions with improved error value is small. This can be explained by the fact that the given MAPE value is already very low for that metric. In other words, we can conclude

that Metric 3 is easy to predict compared to predicting Metric 1, and especially Metric 2. It is seen in Table 9 that there is no evidence to conclude that ERC method is superior to ST method in predicting Metric 1 and 3, since the p-values for the test statistic for comparing residual vectors for ERC and ST are larger than the conventional significance level threshold 0.05. On the other hand, result for Metric 2 conveys a different message. It is seen that prediction performance ERC is significantly better than that of ST at 0.05 significance level.

Table 9: ERC vs ST residuals *t*-test Comparison for testing. \vec{R}_i^j represents residual vector of algorithm *i* for metric *j*.

Residuals	<i>p</i> -Value
$\vec{R}_{ERC}^1 - \vec{R}_{ST}^1$	0.115
$\vec{R}_{ERC}^2 - \vec{R}_{ST}^2$	0.025
$\vec{R}_{ERC}^3 - \vec{R}_{ST}^3$	0.382

In the second phase of the analysis, the effect of the ERC approach on predictive performance is measured for “unusual” dataset. Since this piece of the dataset is outside of the general production characteristics, it is obvious that the regression models which are trained by the data that has usual production parameters will give worse results for this set.

The results of Metric 2, which are already relatively poor, will be worsened for the “unusual” data segment. However, with ERC approach, the unveiled internal relations between target and input variables provide some improvement in the prediction accuracy. Comparison results are presented in Table 10, Table 11 and Table 12.

It is seen in MAPE comparison table that ERC approach provides %6.9, %8 improvement for Metric 1 and 2, respectively. The apparent superiority of the ERC approach compared to the ST is clearly seen in vector comparisons as well. For Metric 2, ST beats ERC in prediction of only 29 samples, whereas the ERC beats ST in 51 samples. It is seen in Table 12 if the significance level is chosen to be 0.1, then ERC dominates ST in all three metrics. On the other hand, when the significance level is set to 0.05, then we may say there is not enough evidence to conclude that ERC method is superior to ST method in predicting Metric 3. However, for Metric 1 and 2, ERC significantly outperforms in ST approach even at 0.05 threshold.

As the final analysis, we present residual vs. fitted plots for i) ST and ERC models (for Metric 2 under “normal” test dataset) in Figure 7 and Figure 8; and ii) ST and ERC models (for Metric 2 under “unusual” test dataset) in Figure 9 and Figure 10. Residual analyses of ST and ERC for other metrics (for both normal and unusual test datasets) are behaving similar char-

acteristics.

Table 10: ERC vs ST Mape Comparison for unusual segment.

	ERC	ST
Metric 1	0.027	0.029
Metric 2	0.127	0.138
Metric 3	0.004	0.004

Table 11: ERC vs ST Vector Comparison for unusual segment.

	ERC	ST
Metric 1	43	37
Metric 2	51	29
Metric 3	44	36

Table 12: ERC vs ST residuals *t*-test Comparison for unusual segment.

Residuals	<i>p</i> -Value
$\vec{R}_{ERC}^1 - \vec{R}_{ST}^1$	0.006
$\vec{R}_{ERC}^2 - \vec{R}_{ST}^2$	0
$\vec{R}_{ERC}^3 - \vec{R}_{ST}^3$	0.078

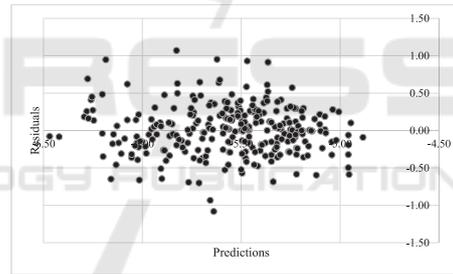


Figure 7: ST-Prediction vs Residuals for Metric 2 in testing.

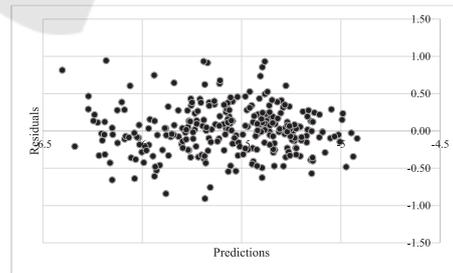


Figure 8: ERC-Prediction vs Residuals for Metric 2 in testing.

It is seen in Figure 7 and Figure 10 that residuals are scattered randomly around mean zero with constant variance. This indicates that both predictive models are adequate in modeling the variation in the response variables in “normal” test data.

Similar to the above discussion, it is seen Figure 7 and Figure 10 that residuals can be assumed to have

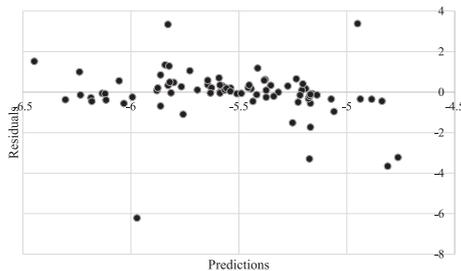


Figure 9: ST-Prediction vs Residuals for Metric 2 in unusual segment.

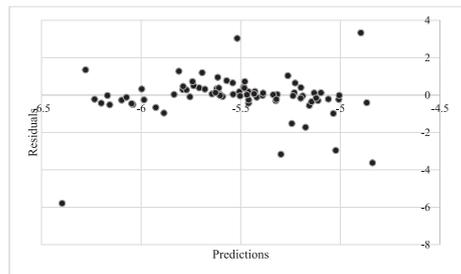


Figure 10: ERC-Prediction vs Residuals for Metric 2 in unusual segment.

zero mean value and show a constant variation behaviour, which is again can be seen as an indication that both predictive models are adequate in modeling the variation in the response variables in "unusual" test data. Although we observe some outliers in the residuals, we could say that this is normal considering that the "unusual" dataset is statistically different than the dataset we train our machine learning algorithms.

4 CONCLUSION

In this paper we proposed an ensemble machine learning algorithm in order to predict the finished yarn quality. The data is first segmented into ten clusters nine of which is denoted as "normal" and the one with the highest distance from the general mean as "unusual" via local outlier factor method. The former cluster refers to production data one may expect due to the nature of the process and latter is the dataset showing an usual pattern compared to expected process data. Then a set of classical machine learning algorithms are applied and performances of the algorithms is compared. It is seen that for the unusual segment, performance of the classical algorithms gets worse especially for one of the quality metrics. As a remedy, an ensemble algorithm based on regressor chains is recommended and yielding higher prediction performance in two thirds of the dataset.

As the next step, implemented algorithm will be

fully tested at the facility. If the prediction performance remains satisfactory, we're going to move on the next phase and start using the predictive tool as a recommendation engine for the machine operator. At this stage, operator will be informed about the suggested production settings for the machine and the recommendation system will perform as a decision support tool, meaning that the recommendations of the tool are push forward to the machine only if the operator gives consent. Once the second phase is successful, the recommendation engine will be plugged into PLC and start changing set parameters of the machine as a part of the automation system. After the third phase, the manufacturing plant will have its first full-scale industry 4.0 application.

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